

Gel'fand–Yaglom type equations for calculating fluctuations around instantons in stochastic systems

Timo Schorlepp^{1,*} , Tobias Grafke²  and Rainer Grauer¹ 

¹ Institute for Theoretical Physics I, Ruhr-University Bochum, Universitätsstrasse 150, D-44801 Bochum, Germany

² Mathematics Institute, University of Warwick, Coventry CV4 7AL, United Kingdom

E-mail: Timo.Schorlepp@rub.de, T.Grafke@warwick.ac.uk and grauer@tp1.rub.de

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Abstract

In recent years, instanton calculus has successfully been employed to estimate tail probabilities of rare events in various stochastic dynamical systems. Without further corrections, however, these estimates can only capture the exponential scaling. In this paper, we derive a general, closed form expression for the leading prefactor contribution of the fluctuations around the instanton trajectory for the computation of probability density functions of general observables. The key technique is applying the Gel'fand–Yaglom recursive evaluation method to the suitably discretized Gaussian path integral of the fluctuations, in order to obtain matrix evolution equations that yield the fluctuation determinant. We demonstrate agreement between these predictions and direct sampling for examples motivated from turbulence theory.

Keywords: instanton calculus, fluctuation determinant, large deviation theory

(Some figures may appear in colour only in the online journal)

1. Introduction

Quantifying the probability of rare events is extraordinarily difficult: they are usually too rare to be efficiently observed or sampled, and at the same time too important to be ignored. A

* Author to whom any correspondence should be addressed.



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traditional approach in statistical physics is to phrase the problem as a path integral, and extract scaling information from a saddle point approximation (‘instanton’ approximation).

Saddle point techniques have their origin in solid state and quantum physics [1–3], where also the term ‘instanton’ was introduced. The close relation to large deviation theory was reviewed in [4], and its role as a non-perturbative method to evaluate path integrals in [5, 6].

The instanton calculus consists of four steps: first, the instanton is computed as the classical solution that minimizes the corresponding action. This step already quantifies the exponential scaling behavior of the probability density function (PDF) under consideration. Second, the contribution of fluctuations is taken into account by expanding the action to second order around the instanton, which yields a Gaussian path integral. This contribution corresponds to the fluctuation determinant of the second variation of the instanton action. Depending on the system at hand, as third and fourth step, one needs to consider continuous symmetries (zero modes) and the instanton gas, respectively.

Recently, there has been much activity and progress in numerous stochastic dynamical systems on the first step, such as the Kardar–Parisi–Zhang equation [7], Ginzburg–Landau equation [8], Earth’s climate [9], biofilm formation [10] and ocean surface waves [11], but, except for the recent paper [12], progress on the remaining steps is developed only for specific applications [13, 14]. In this paper, we focus on the second step and develop a general formalism to compute the contributions of quadratic fluctuations around the instanton solution to the path integral for the evaluation of PDFs. We will present our approach for general finite dimensional Langevin equations, but with the focus that the developed methods are (in particular numerically) applicable to large systems of stochastic ordinary differential equations (SDEs) and finally to stochastic partial differential equations (SPDEs) relevant in fluid and plasma turbulence (e.g. Burgers, Navier–Stokes and the magnetohydrodynamic equations). The computation of fluctuations around instantons is the most important issue in developing a non-perturbative approach to understanding anomalous scaling in turbulence.

The outline of this paper is as follows: in section 2, we summarize the path integral formulation of stochastic systems, introduce the instanton solutions, and clarify the connection with large deviation theory. Section 3 is the central part of this work that contains our approach to calculating the fluctuation determinant. The main technical issues that we address in this section are the calculation of the marginal distribution by performing an appropriate integral over all permitted boundary conditions of the fluctuations, and the impact of the discretization of the path integral on the fluctuation matrix and its determinant in particular. This leads to equations of the Gel’fand–Yaglom type, which can be linearized by a Radon transformation. The resulting simple equations allow the calculation of the fluctuation determinant even for large systems of SDEs and ultimately also SPDEs. In section 4, we present multiple examples to validate our method and compare its predictions to analytically known results as well as Monte Carlo simulations. We conclude the paper with a short discussion of our results in section 5.

2. Instantons and large deviations

Consider the stochastic differential equation (SDE)

$$\dot{u} + N(u) = \eta, \quad u(-T) = u_0, \quad (1)$$

where the state of the system is described by the vector $u \in \mathbb{R}^d$ on the time interval $[-T, 0]$ (for $T > 0$), and the initial value $u_0 \in \mathbb{R}^d$ is deterministic. The (possibly nonlinear) deterministic term $N : \mathbb{R}^d \mapsto \mathbb{R}^d$ will be referred to as the *drift term*, while stochasticity is introduced via

the d -dimensional white-in-time Gaussian noise η with covariance $\chi \in \mathbb{R}^{d \times d}$ and amplitude $\varepsilon > 0$,

$$\langle \eta_i(t) \eta_j(t') \rangle = \varepsilon \chi_{ij} \delta(t - t'). \quad (2)$$

Here, $\langle \cdot \rangle$ denotes the ensemble average over noise realizations. We are interested in the small noise limit $\varepsilon \rightarrow 0$, for which the dynamics given by (1) are a perturbation of the deterministic dynamics

$$\dot{u} = -N(u), \quad u(-T) = u_0, \quad (3)$$

which we further assume to have a single fixed point \bar{u} , the basin of attraction of which covers all of \mathbb{R}^d . Note that we consider χ to be independent of u , which corresponds to additive Gaussian noise.

Now, we are interested in (possibly nonlinear) *observables* of the form $O : \mathbb{R}^d \mapsto \mathbb{R}^{d'}$ which represent some quantities of interest that we wish to measure at the end of our time interval at $t = 0$. For example, we might want to focus on one component of our final state, or on its average (both cases would have $d' = 1$). Due to the presence of the noise, the observable $O(u(0))$ is a random variable, and we might want to talk about its PDF ρ_O . In particular, as is common in stochastic field theory, the PDF of the observable can be written as a path integral. As we will discuss next, the small noise limit, $\varepsilon \rightarrow 0$, then corresponds to a semi-classical limit of this path integral, allowing for an estimate via saddlepoint approximation and evaluation of the fluctuation determinant.

Remark 1 In certain applications, one does not actually take the small noise limit $\varepsilon \rightarrow 0$, but considers a fixed noise strength which may correspond e.g. to a given Reynolds number in fluid turbulence. Then, in this setup, one usually focuses on the tails of the PDF ρ_O at this specific strength of forcing and estimates the tail scaling of the PDF using the instanton method. In this paper, we will exclusively focus on the small noise limit in order to be able to perform a clean expansion in ε . However, we remark that for SPDEs with certain scaling invariances, such as the Burgers or Navier–Stokes equation, these two limits, i.e. small noise and large observable amplitude, strictly correspond to each other by a suitable rescaling of all variables. For concreteness, consider the one-dimensional stochastic Burgers equation in terms of physical quantities

$$\partial_t u + u \partial_x u - \nu \partial_{xx} u = \eta, \quad \langle \eta(x, t) \eta(x', t') \rangle = \chi(x - x') \delta(t - t'), \quad (4)$$

and take the gradient at one point in space and time

$$O(u(\cdot, t = 0)) = \partial_x u(x = 0, t = 0), \quad (5)$$

as the observable of interest. Now suppose we want to estimate the PDF of this observable at a large observable value of

$$|\partial_x u(x = 0, t = 0)| = a_0. \quad (6)$$

In general, the Burgers equation can be non-dimensionalized by introducing a characteristic length scale x_0 , a characteristic time scale t_0 and a consistent velocity scale $u_0 = x_0/t_0$ as well as a characteristic strength of the forcing χ_0 :

$$\tilde{x} = \frac{x}{x_0}, \quad \tilde{t} = \frac{t}{t_0}, \quad \tilde{u} = \frac{u}{u_0}, \quad \tilde{\eta} = \eta \frac{t_0^{1/2}}{\chi_0}. \quad (7)$$

Dropping all tildes, the Burgers equation in terms of non-dimensionalized quantities reads

$$\partial_t u + u \partial_x u - \text{Re}^{-1} \partial_{xx} u = \frac{\chi_0^{1/2} t_0^{1/2}}{u_0} \eta, \quad \langle \eta(x, t) \eta(x', t') \rangle = \chi(x - x') \delta(t - t'), \quad (8)$$

with the Reynolds number $\text{Re} = u_0 x_0 / \nu$. Adapting the time scale to the gradient strength via

$$a_0 \stackrel{!}{=} \frac{u_0}{x_0} = \frac{1}{t_0}, \quad (9)$$

and choosing $x_0 = \sqrt{\nu/a_0}$ then leads to

$$\partial_t u + u \partial_x u - \partial_{xx} u = \eta, \quad \langle \eta(x, t) \eta(x', t') \rangle = \varepsilon \chi(x - x') \delta(t - t'), \quad (10)$$

with the noise strength

$$\varepsilon = \frac{\chi_0}{\nu} \cdot \frac{1}{a_0^2} \xrightarrow{a_0 \rightarrow \infty} 0, \quad (11)$$

as the only dimensionless control parameter, which corresponds precisely to the small noise limit that will be treated in the remainder of the paper.

2.1. Path integral

Formally, the PDF of the observable O can be expressed as

$$\rho_O(a) = \langle \delta(O(u(0)) - a) \rangle. \quad (12)$$

We can write this as a path integral over all noise realizations η via

$$\rho_O(a) = \int D\eta \delta(O(u[\eta](0)) - a) \exp \left\{ -\frac{1}{2\varepsilon} \int_{-T}^0 dt (\eta, \chi^{-1} \eta)_d \right\}, \quad (13)$$

where the suitably normalized path density of noise realizations is given by the Gaussian term, and we introduced the \mathbb{R}^d inner product abbreviated by $(\cdot, \cdot)_d$. The η -dependence of the final configuration $u(0)$ is denoted here explicitly as $u[\eta](0)$.

For convenience, we can perform a change of variables from noise realizations η to field realizations u by inserting the SDE (1) itself,

$$\begin{aligned} \rho_O(a) &= \int Du J(u) \delta(O(u(0)) - a) \\ &\quad \times \exp \left\{ -\frac{1}{2\varepsilon} \int_{-T}^0 dt (\dot{u} + N(u), \chi^{-1} (\dot{u} + N(u)))_d \right\}. \end{aligned} \quad (14)$$

The Jacobian associated with this change of variables, together with a careful treatment of the continuum limit of the stochastic path integral [15], introduces an additional term $J(u)$ in the prefactor, which will be important later when dealing with the corrections from fluctuations. For now, we focus on the exponential term of order ε^{-1} representing the *action functional* $S[u]$ denoted by

$$S[u] = \frac{1}{2} \int_{-T}^0 dt \mathcal{L}(u, \dot{u}) = \frac{1}{2} \int_{-T}^0 dt (\dot{u} + N(u), \chi^{-1} (\dot{u} + N(u)))_d, \quad (15)$$

where we call $\mathcal{L}(u, \dot{u})$ the *Lagrangian*. Written in this form, the action functional corresponds to the classical *Onsager–Machlup* action [16] of the stochastic process (1).

For many applications of relevance, the noise covariance χ is not necessarily invertible, corresponding to degrees of freedom of the system that are unforced. This kind of *degenerate forcing* renders the above formalism unwieldy, as terms involving χ^{-1} must be treated with care. A standard way to overcome this complication was proposed by Janssen and de Dominicis [17, 18] by introducing an additional *response field* p via

$$\chi p = \dot{u} + N(u). \quad (16)$$

With this transformation, the Onsager–Machlup action (15) is changed into the Janssen-de Dominicis action

$$S[u, p] = \int_{-T}^0 dt \left((p, \dot{u} + N(u))_d - \frac{1}{2} (p, \chi p)_d \right) = \frac{1}{2} \int_{-T}^0 dt (p, \chi p)_d. \quad (17)$$

Written like that, the response field can be interpreted as the *conjugate momentum* of the field variable u . Note that we formally set the action to infinity if $(\dot{u} + N(u))$ lies in the kernel of χ . This simply corresponds to the fact that trajectories $u(t)$ which are impossible to realize with our degenerate forcing are assigned zero probability. Note also that in the following derivations, we will treat χ as invertible, but the final result will be formulated only in terms of χ itself. The derivation remains valid if one were to take the singular limit carefully.

2.2. Instantons

The evaluation of the path integral (14) is a non-trivial task in general. In the small noise limit, $\varepsilon \rightarrow 0$, though, we can make use of a saddlepoint approximation, expanding the action functional around its minimum. In effect, this corresponds to an infinite dimensional Laplace method to approximate the path integral. It is noteworthy that this expansion is non-perturbative with respect to the original SDE (1), i.e. taking every nonlinearity fully into account. Instead, it corresponds to an expansion around the most likely pathway u_I , the classical trajectory, also called the *instanton*, for which $\delta S[u_I] = 0$.

More concretely, the instanton is defined as the solution to the constrained optimization problem

$$u_I = \arg \min_{\substack{u(-T)=u_0 \\ O(u(0))=a}} S[u]. \quad (18)$$

A standard way to solve this constrained optimization problem is by introducing a Lagrange multiplier $\mathcal{F} \in \mathbb{R}^{d'}$ to ensure the constraint $O(u(0)) = a$ at the final point $t = 0$, to obtain

$$\tilde{S}[u] := S[u] + (\mathcal{F}, O(u(0)) - a)_d. \quad (19)$$

When considering this in the Janssen–de Dominicis framework, with $\chi p = \dot{u} + N(u)$, the first order variation of \tilde{S} is given by

$$\begin{aligned} \tilde{S}[u + \delta u] &= S[u] + \int_{-T}^0 dt \left[(\delta u, -\dot{p} + \nabla N(u)^\top p)_d \right] \\ &\quad + (\delta u(0), p(0) + \nabla O(u(0))^\top \mathcal{F})_d. \end{aligned} \quad (20)$$

At the trajectory (u_1, p_1) of vanishing first variation we obtain the *instanton equations*

$$\begin{cases} \dot{u}_1 + N(u_1) = \chi p_1 & u_1(-T) = u_0 \\ \dot{p}_1 - \nabla N(u_1)^\top p_1 = 0 & p_1(0) = -\nabla O(u_1(0))^\top \mathcal{F}_1 \end{cases}. \quad (21)$$

The action at the instanton as a function of the observable value a , denoted by $S_1(a)$ is therefore given by

$$S_1(a) := S[u_1] = \frac{1}{2} \int_{-T}^0 dt (p_1, \chi p_1)_d. \quad (22)$$

At this point, if we are able to find the instanton (u_1, p_1) as solution of the constrained minimization problem (18), then we have access to the *exponential scaling* of the PDF of our observable via

$$\rho_O(a) = Z_\varepsilon(a) e^{-\varepsilon^{-1} S_1(a)}, \quad (23)$$

for a prefactor component Z_ε that might still depend on a . It is the goal of the following sections to obtain a set of equations to compute also, for each a and as $\varepsilon \rightarrow 0$, the prefactor $Z_\varepsilon(a)$ to leading order in ε (the result of which we denote by $Z(a)$) in order to obtain the full probability density $\rho_O(a)$ with

$$\rho_O(a) \stackrel{\varepsilon \rightarrow 0}{\sim} Z(a) e^{-\varepsilon^{-1} S_1(a)}. \quad (24)$$

Remark 2 The above considerations are equivalent to sample path large deviation theory, and in particular Freidlin–Wentzell theory [19]. In particular, the action functional given in equation (15) corresponds exactly to the Freidlin–Wentzell rate function for sample paths.

3. The contribution of the quadratic fluctuations

In this section we derive a general prescription that permits the computation of the PDF prefactor Z from (24) for any Langevin-type SDE (1) with additive noise in the small noise limit $\varepsilon \rightarrow 0$. Concretely, we will show that to leading order (in ε) the PDF can be approximated by

$$\begin{aligned} \rho_O(a) &= (2\pi\varepsilon)^{-d'/2} \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt \operatorname{tr} [(\nabla \nabla N(u_1(t)), p_1(t))_d Q(t)] \right\} \\ &\quad \times [\det U \det (\nabla O(u_1(0)) Q(0) U^{-1} \nabla O(u_1(0))^\top)]^{-1/2} \exp \{-\varepsilon^{-1} S_1\}. \end{aligned}$$

Here, the prefactor depends on the solution $Q : [-T, 0] \mapsto \mathbb{R}^{d \times d}$ of a matrix Riccati equation

$$\dot{Q} = \chi - Q \nabla N^\top(u_1) - \nabla N(u_1) Q - Q(\nabla \nabla N(u_1), p_1)_d Q, \quad Q(-T) = 0,$$

to be evaluated along the instanton trajectory (u_1, p_1) , and U denotes the $d \times d$ matrix

$$U = 1 + (\nabla \nabla O(u_1(0)), \mathcal{F}_1)_{d'} Q(0).$$

Intuitively, the prefactor term quantifies the functional determinant of the second variation of the action functional, which can be computed by the evaluation of the Gaussian path integral representing the fluctuations around the instanton trajectory. The Riccati equation is then equivalent to an evaluation of the functional determinant by the Gel'fand–Yaglom method.

It is well known, and has been discussed at length in the 1970s and 1980s in the literature [15, 20–23], that a correct and consistent discretization of the stochastic path integral is necessary in order to obtain meaningful results. This is due to the fact that the fluctuations in the quadratic expansion constitute a Gaussian stochastic process which is almost surely nondifferentiable, so the rules of stochastic calculus have to be applied if calculations involving the fluctuations are done in the continuum limit. While the SDE (1) has additive noise and hence always describes the same stochastic process, independent of the specific stochastic calculus in terms of which is interpreted, one has to be more careful when performing path integral calculations. Consequently, we will carry out all derivations in a discretized setting and comment specifically on all instances where the continuum limit is taken. Prior to this detailed discrete derivation, we briefly discuss some general aspects of the quadratic expansion in the continuum limit to give an overview, and also comment on how to evaluate the prefactor numerically by Monte Carlo methods.

3.1. Overview in the continuum limit

In continuum notation (14), the PDF of $O(u(t=0))$ can be written as

$$\begin{aligned} \rho_O(a) = & \int_{u(-T)=u_0} Du \, \delta(O(u(0)) - a) \exp \left\{ \frac{1}{2} \int_{-T}^0 dt \, \text{tr} [\nabla N(u)] \right. \\ & \left. - \frac{1}{2\varepsilon} \int_{-T}^0 dt (\dot{u} + N(u), \chi^{-1} [\dot{u} + N(u)]_d)_d \right\}, \end{aligned} \quad (25)$$

where we explicitly included the term of order ε^0 for the generalized Onsager–Machlup action in the continuum limit. Once the instanton trajectory u_I given by (18) has been found, we insert

$$u = u_I + \sqrt{\varepsilon} \delta u \quad (26)$$

in the path integral in order to expand the action around the instanton, where δu will be referred to as the *fluctuations* around the instanton. In the small noise limit $\varepsilon \rightarrow 0$, this expansion then leads to a Gaussian path integral (details can be found in the next section)

$$\begin{aligned} \rho_O(a) & \stackrel{\varepsilon \rightarrow 0}{\sim} \varepsilon^{-d'/2} \exp \{ -\varepsilon^{-1} S_I(a) \} \int_{\delta u(-T)=0} D(\delta u) \, \delta(\nabla O(u_I(0)) \delta u(0)) \\ & \times \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt (\delta u, (\nabla \nabla N(u_I), p_I)_d \delta u)_d \right\} \\ & \times \exp \left\{ -\frac{1}{2} (\delta u(0), (\nabla \nabla O(u_I(0)), \mathcal{F}_I)_d \delta u(0))_d \right\} \\ & \times \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt (\delta \dot{u} + \nabla N(u_I) \delta u, \chi^{-1} [\delta \dot{u} + \nabla N(u_I) \delta u]_d)_d - \text{tr} [\nabla N(u_I)] \right\}, \end{aligned} \quad (27)$$

where $(\nabla \nabla N(u_I), p_I)_d$ is a shorthand notation for the $d \times d$ matrix

$$[(\nabla \nabla N(u_I), p_I)_d]_{kl} = (\partial_k \partial_l N(u_I), p_I)_d. \quad (28)$$

Hence, we see that in a probabilistic sense, the prefactor is given by the expectation

$$Z = \varepsilon^{-d'/2} \left\langle \delta(\nabla O(u_I(0))\delta u(0)) \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt (\delta u, (\nabla \nabla N(u_I), p_I)_d \delta u)_d \right\} \right. \\ \left. \times \exp \left\{ -\frac{1}{2} (\delta u(0), (\nabla \nabla O(u_I(0)), \mathcal{F}_I)_d \delta u(0))_d \right\} \right\rangle, \quad (29)$$

where δu is a d -dimensional Gaussian process on $[-T, 0]$ with $\delta u(-T) = 0$ that satisfies the linear SDE

$$\delta \dot{u} + \nabla N(u_I) \delta u = \eta, \quad \langle \eta(t) \eta^\top(t') \rangle = \chi \delta(t - t'). \quad (30)$$

Of course this expectation could be evaluated by Monte Carlo simulations of the SDE (30), but this suffers from the usual drawbacks of Monte Carlo methods, and we aim at developing a closed form deterministic expression for Z instead, that is also cheap to evaluate numerically. However, in our numerical examples, this possibility to compute the prefactor provides a good benchmark for our analytical results.

Remark 3 If the drift term N and observable O are polynomials, then the expansion of the action around the instanton will terminate at a finite order, without considering the small noise limit $\varepsilon \rightarrow 0$. For concreteness, consider a quadratic drift term and a linear observable, which is again relevant e.g. for the Burgers equation. Then, upon expanding the action in (25), we see that the full prefactor Z_ε for $\varepsilon > 0$, which we define by (23), will still be given by the expectation in (29) (without the $\nabla \nabla O$ -term), but now δu fulfills the nonlinear SDE

$$\delta \dot{u} + \nabla N(u_I) \delta u + \frac{\sqrt{\varepsilon}}{2} (\delta u, \nabla \nabla N(u_I) \delta u)_d = \eta, \quad \langle \eta(t) \eta^\top(t') \rangle = \chi \delta(t - t'), \quad (31)$$

where we explicitly see the influence of non-Gaussian fluctuations for finite ε . Performing Monte Carlo simulations of (31) in order to compute the full prefactor outside of the small noise limit corresponds to importance sampling of the original SDE (1) using the instanton. We call this procedure instanton based importance sampling (ibis [24]) and will use it in our numerical experiments in order to compare the quadratic and full prefactor.

Now, our task in this section is to evaluate the Gaussian path integral (27). What renders the problem non-standard are the final time boundary conditions and terms: $\delta u(t = 0)$ is constrained to the kernel of $\nabla O(u_I(t = 0))$. This corresponds to the situation where possible (infinitesimal) final fluctuations are confined to the directions in which the value of our observable remains invariant. We explicitly have to integrate over all boundary conditions of this subspace of \mathbb{R}^d (and these boundary conditions also enter the final result via the $\nabla \nabla O$ -term for nonlinear observables). We will present two alternatives to do so in this paper. The first variant consists of integrating out the degrees of freedom on the final time boundary in order to reduce the remaining fluctuation path integral to Dirichlet 0 boundary conditions. We term this procedure the *homogenization* of the boundary conditions of the fluctuation determinant.

The determination of the remaining functional determinant with Dirichlet 0 boundary conditions of the second variation operator

$$H = (\nabla \nabla N(u_I), p_I)_d + \left[-\frac{d}{dt} + \nabla N(u_I)^\top \right] \chi^{-1} \left[\frac{d}{dt} + \nabla N(u_I) \right] \quad (32)$$

from (27) is then a standard procedure, and we explicitly derive Gel'fand–Yaglom like equations for the evaluation of this determinant. An aspect that has not yet been discussed

in detail in the literature to our best knowledge is the dependence of these Gel'fand–Yaglom equations on the discretization of the path integral in the continuum limit. In particular, the functional determinant *does* indeed depend on the discretization, and it is only the Jacobian term from the noise-to-field transformation that cancels this discretization dependence and renders the final result independent of the discretization choice. For the Gel'fand–Yaglom equation, we therefore have a freedom of choice of the discretization, as long as we correct this with the correct corresponding Jacobian. For this reason, we are able to choose the discretization optimal for computational purposes. We also remark that there already exists a large body of literature that discusses Gel'fand–Yaglom type equations in a more functional analytic setting, important references being [25, 26]. A useful review is provided by [27]. In this setup, one usually considers quotients of functional determinants or regularization procedures such as zeta function regularization in order to obtain well defined results, and we prefer to work out the straightforward discretization approach in this paper (see, however, the related paper [28], where the prefactor of the work distribution in one-dimensional Langevin systems is calculated directly by adopting the results of Kirsten and McKane [26] obtained by applying contour integration methods to the zeta function of the respective Sturm–Liouville operators).

After following through with this program, we will have obtained a Gel'fand–Yaglom formula and boundary homogenization procedure that leads to a closed form representation of the prefactor contributions. Finally, we will derive the representation of the PDF prefactor without homogenization of the boundary conditions that has been stated at the beginning of this section and can more easily be computed for large system dimensions d . In the context of hydrodynamic shell models, Daumont *et al* [13] have derived a related expression for the influence of the quadratic fluctuations on the PDF prefactor of a one-dimensional observable by path integral calculations, but their derivation lead to a more complicated procedure, which they also did not discuss in the continuum limit. Furthermore, Dean, Miao and Podgornik have derived a similar expression involving algebraic Riccati equations in the case of constant coefficients in [29] via the Feynman–Kac formula. We adapt their derivation to our problem in remark 4.

3.2. Quadratic expansion of the discrete action

The starting point of our derivation is a time-discretized version of (1): for $\alpha \in [0, 1]$ and $n \in \mathbb{N}$, consider

$$\frac{u_{i+1} - u_i}{\Delta t} + \alpha N(u_{i+1}) + (1 - \alpha)N(u_i) = \eta_i, \quad i = 0, \dots, n-1, \quad (33)$$

with $\Delta t = T/n$. Here, u_0 is still chosen deterministically from the initial condition of (1), and u_1, \dots, u_N are \mathbb{R}^d -valued random variables. The discretized white noise consists of n zero-mean, \mathbb{R}^d -valued Gaussian random variables $\eta_0, \dots, \eta_{n-1}$ with

$$\langle \eta_i \eta_j^\top \rangle = \frac{\varepsilon}{\Delta t} \chi \delta_{ij}. \quad (34)$$

The parameter α of the discretization interpolates between the explicit Euler–Maruyama method for $\alpha = 0$ and the fully implicit choice $\alpha = 1$. We stress again that any choice of α has to yield the same continuum limit, and we will use this freedom to make a computationally optimal choice later on. Now, with this discretization, the PDF of $O(u(0))$, evaluated at $a \in \mathbb{R}^{d^f}$, can be written as

$$\rho_O(a) = \lim_{n \rightarrow \infty} \langle \delta(O(u_n) - a) \rangle \quad (35)$$

$$\begin{aligned} &= \lim_{n \rightarrow \infty} \left(\frac{\Delta t}{2\pi\varepsilon} \right)^{nd/2} (\det \chi)^{-n/2} \int_{\mathbb{R}^d} \left(\prod_{i=0}^{n-1} d^d \eta_i \right) \delta(O(u_n) - a) \\ &\quad \times \exp \left\{ -\frac{\Delta t}{2\varepsilon} \sum_{i=0}^{n-1} (\eta_i, \chi^{-1} \eta_i)_d \right\}. \end{aligned} \quad (36)$$

The next step is to perform a substitution in the integral in order to be able to integrate over the field u itself. The discrete transformation rule (33) from $\eta_0, \dots, \eta_{n-1}$ to u_1, \dots, u_n yields the discretization-dependent Jacobian

$$\begin{aligned} J_\alpha^{(n)}[u] &= \det \left[\left(\frac{\partial \eta_i}{\partial u_j} \right)_{\substack{i=0, \dots, n-1 \\ j=1, \dots, n}} \right] \\ &= \Delta t^{-nd} \det \left[\prod_{i=n-1}^0 (1 + \alpha \Delta t \nabla N(u_{i+1})) \right]. \end{aligned} \quad (37)$$

In the continuum limit $n \rightarrow \infty$, $\Delta t \rightarrow 0$, this term asymptotically behaves as

$$J_\alpha^{(n)}[u] \stackrel{n \rightarrow \infty}{\sim} \Delta t^{-nd} \exp \left\{ \alpha \int_{-T}^0 \text{tr} [\nabla N(u(t))] dt \right\}, \quad (38)$$

which can easily be seen by noting that the product in (37) tends to the solution of the matrix differential equation

$$\dot{M}(t) = \alpha \nabla N(u(t)) M(t), \quad M(-T) = 1 \in \mathbb{R}^{d \times d}, \quad (39)$$

so its determinant satisfies

$$\frac{d}{dt} \det M(t) = \alpha \text{tr} [\nabla N(u(t))] \det M(t), \quad \det M(-T) = 1, \quad (40)$$

by virtue of the general identity

$$\frac{d}{dt} \det M(t) = \det M(t) \text{tr} [M(t)^{-1} \dot{M}(t)]. \quad (41)$$

Two important observations regarding the Jacobian (38) are to be made: firstly, the exponent is $\mathcal{O}(\varepsilon^0)$, so it is of no importance for the computation of the instanton field itself in the small noise limit, and secondly, we can consequently naively substitute its continuum limit everywhere in the following. The PDF (35) after the $\eta \rightarrow u$ substitution thus reads

$$\begin{aligned} \rho_O(a) &= \lim_{n \rightarrow \infty} (2\pi\varepsilon\Delta t)^{-nd/2} (\det \chi)^{-n/2} \int_{\mathbb{R}^d} \left(\prod_{j=1}^n d^d u_j \right) \delta(O(u_n) - a) \\ &\quad \times \exp \left\{ \alpha \int_{-T}^0 \text{tr} [\nabla N(u(t))] dt \right\} \exp \left\{ -\varepsilon^{-1} S^{(n)}[u] \right\}, \end{aligned} \quad (42)$$

where the discretized Onsager–Machlup action is denoted by

$$S^{(n)}[u] = \frac{\Delta t}{2} \sum_{i=0}^{n-1} \left(\frac{u_{i+1} - u_i}{\Delta t} + \alpha N(u_{i+1}) + (1 - \alpha) N(u_i), \chi^{-1}[\dots] \right)_d, \quad (43)$$

where $[\dots]$ is a placeholder for the repetition of the left argument of the inner product. For this discrete action at order $\mathcal{O}(\varepsilon^{-1})$, we then have to compute the discrete instanton $u_{1,0}, \dots, u_{1,n}$ which minimizes the action under the boundary condition $O(u_{1,n}) = a$, and its corresponding conjugate momentum $p_{1,0}, \dots, p_{1,n}$. The method of Lagrange multipliers as explained in section 2.2 can explicitly be incorporated in the path integral by using the identity

$$\delta(f(x)) = \frac{1}{(2\pi)^{d'}} \int_{\mathbb{R}^{d'}} d^{d'} k \exp \{i(k, f(x))_{d'}\}, \quad (44)$$

or, with $\mathcal{F} = ik\varepsilon$,

$$\begin{aligned} \rho_O(a) &= \lim_{n \rightarrow \infty} (2\pi\varepsilon\Delta t)^{-nd/2} (\det \chi)^{-n/2} (2\pi i\varepsilon)^{-d'} \int_{\mathbb{R}^{d'}} d^{d'} \mathcal{F} \\ &\times \int_{\mathbb{R}^d} \left(\prod_{j=1}^n d^d u_j \right) \times \exp \left\{ \alpha \int_{-T}^0 \text{tr} [\nabla N(u(t))] dt \right\} \\ &\times \exp \left\{ -\varepsilon^{-1} (S^{(n)}[u] + (\mathcal{F}, O(u_n) - a)_{d'}) \right\}, \end{aligned} \quad (45)$$

Note that the instanton will typically be a classical (in the sense of at least C^2) minimizer of the action in the continuum limit, so any numerical scheme or discretization can in fact be used to determine the instanton without introducing a systematic error for the following calculations.

Once the instanton has been determined for the specific system at hand, we insert the substitution

$$u_j = u_{1,j} + \sqrt{\varepsilon} \delta u_j, \quad j = 1, \dots, n \quad (46)$$

in the integral (45), where δu_j can be interpreted as the fluctuations around the instanton at time j . Analogously, we substitute

$$\mathcal{F} = \mathcal{F}_1 + \sqrt{\varepsilon} \delta \mathcal{F}, \quad (47)$$

where $\mathcal{F}_1 = \mathcal{F}_1(a)$ is the specific Lagrange multiplier for the solution of the instanton optimization problem (18) with boundary condition $O(u_{1,n}) = a$. Expanding in the small noise limit $\varepsilon \rightarrow 0$ around the instanton trajectory then yields a Gaussian path integral in the fluctuations, which we can explicitly evaluate. Concretely, inserting equations (46) and (47) into the PDF and expanding yields

$$\begin{aligned} \rho_O(a) &= \lim_{n \rightarrow \infty} (2\pi\Delta t)^{-nd/2} (\det \chi)^{-n/2} \exp \left\{ \alpha \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \left\{ -\varepsilon^{-1} S_1(a) \right\} \\ &\times \varepsilon^{-d'/2} \int_{\mathbb{R}^d} \left(\prod_{j=1}^n d^d (\delta u_j) \right) \delta(\nabla O(u_{1,n}) \delta u_n) \\ &\times \exp \left\{ -\delta^2 S^{(n)}[\delta u] - \frac{1}{2} (\delta u_n, (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \delta u_n)_d \right\}, \end{aligned} \quad (48)$$

with the second order expansion of the discretized action given by

$$\begin{aligned} \delta^2 S^{(n)}[\delta u] = & \frac{\Delta t}{2} \left(\sum_{i=0}^{n-1} \left[\left(\frac{\delta u_{i+1} - \delta u_i}{\Delta t} + \alpha \nabla N(u_{1,i+1}) \delta u_{i+1} + (1 - \alpha) \nabla N(u_{1,i}) \delta u_i, \right. \right. \right. \\ & \left. \left. \chi^{-1} \left[\frac{\delta u_{i+1} - \delta u_i}{\Delta t} + \alpha \nabla N(u_{1,i+1}) \delta u_{i+1} + (1 - \alpha) \nabla N(u_{1,i}) \delta u_i \right] \right)_d \right. \\ & \left. + (\delta u_i, (\nabla \nabla N(u_{1,i}), p_{1,i})_d \delta u_i)_d \right] + \alpha (\delta u_n, (\nabla \nabla N(u_{1,n}), p_{1,n})_d \delta u_n)_d \Big), \quad (49) \end{aligned}$$

where we set $\delta u_0 = 0$. The remaining task is to evaluate the Gaussian integral (48) efficiently in the limit $n \rightarrow \infty$.

3.3. Homogenizing the boundary conditions

In this section, we reduce the path integral (48) with boundary constraint $\delta u_n \in \ker \nabla O(u_{1,n})$ to an equivalent problem with Dirichlet 0 boundary conditions $\delta u_n = 0$. In the following, we will assume that the linear map $\nabla O(u_{1,n}) : \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$ has full rank $d' \leq d$ for our notational convenience. We then introduce an orthonormal basis $\{\delta u_n^{(1)}, \dots, \delta u_n^{(d-d')}\}$ of the linear subspace

$$\ker \nabla O(u_{1,n}) \subset \mathbb{R}^d \quad (50)$$

and extend this basis to an orthonormal basis $\{\delta u_n^{(1)}, \dots, \delta u_n^{(d-d')}, v^{(1)}, \dots, v^{(d')}\}$ of \mathbb{R}^d . Writing δu_n in terms of these basis vectors as

$$\delta u_n = \sum_{i=1}^{d-d'} \beta_i \delta u_n^{(i)} + \sum_{j=1}^{d'} \gamma_j v^{(j)}, \quad (51)$$

the fluctuations in the v_i -directions are irrelevant for the boundary integral over δu_n in (48). Therefore, after changing to this basis, we can drop the subspace constraint in (48) and only integrate over the remaining $d - d'$ -dimensional relevant subspace, which yields

$$\begin{aligned} & \int_{\mathbb{R}^d} d^d(\delta u_n) \delta(\nabla O(u_{1,n}) \delta u_n) \exp \left\{ -\delta^2 S^{(n)}(\delta u_0 = 0, \delta u_1, \dots, \delta u_{n-1}, \delta u_n) \right. \\ & \quad \left. - \frac{1}{2} (\delta u_n, (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \delta u_n)_d \right\} \\ & = [\det(\nabla O(u_{1,n}) \nabla O(u_{1,n})^\top)]^{-1/2} \int_{\mathbb{R}^{d-d'}} d^{d-d'} \beta \\ & \quad \times \exp \left\{ -\delta^2 S^{(n)} \left(0, \delta u_1, \dots, \delta u_{n-1}, \sum_{i=1}^{d-d'} \beta_i \delta u_n^{(i)} \right) \right\} \\ & \quad \times \exp \left\{ -\frac{1}{2} \sum_{i,j=1}^{d-d'} \beta_i \beta_j (\delta u_n^{(i)}, (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \delta u_n^{(j)})_d \right\}. \quad (52) \end{aligned}$$

Now, by interchanging the order of integration in (48), the integral can be interpreted in the sense that for each individual, *fixed* boundary condition

$$\delta u_n^* = \sum_{i=1}^{d-d'} \beta_i^* \delta u_n^{(i)}, \quad (53)$$

the remaining $(d \cdot (n-1))$ -dimensional integral over the integrand

$$\exp \left\{ -\delta^2 S^{(n)}(\delta u_0 = 0, \delta u_1, \dots, \delta u_{n-1}, \delta u_n^*) \right\}, \quad (54)$$

has to be carried out for this particular boundary condition. What we propose to do is to perform, for each fixed boundary condition δu_n^* , a shift in the other integration variables:

$$\delta u_i = \delta u_i^* + \delta \tilde{u}_i, \quad u = 1, \dots, n-1, \quad (55)$$

such that integration is then performed over $(\delta \tilde{u}_i)_{1 \leq i \leq n-1}$ instead and we demand that

$$\begin{aligned} & \delta^2 S^{(n)}(\delta u_0 = 0, \delta u_1, \dots, \delta u_{n-1}, \delta u_n^*) \\ & \stackrel{!}{=} \delta^2 S^{(n)}(0, \delta u_1^*, \dots, \delta u_{n-1}^*, \delta u_n^*) + \delta^2 S^{(n)}(0, \delta \tilde{u}_1, \dots, \delta \tilde{u}_{n-1}, 0). \end{aligned} \quad (56)$$

Effectively, this corresponds to the condition that the first order variation (with fixed end points) of the quadratic action should vanish at the δu_i^* -trajectory, so we compute additional instantons for each of the given boundary condition δu_n^* . If this cannot be solved analytically, it is of course hopeless to do this numerically for every single boundary condition, but, since the action is quadratic at this stage, it suffices to determine these δu_i^* trajectories once for each of the basis vectors $\delta u^{(1)}, \dots, \delta u^{(d-d')}$. In the continuum limit, which can again be taken naively for these additional, differentiable instantons, the condition (56) can be written in terms of a linear boundary value problem (BVP)

$$\begin{cases} \frac{d}{dt} \begin{pmatrix} \delta u \\ \delta p \end{pmatrix} = \begin{pmatrix} -\nabla N(u_1) & \chi \\ (\nabla \nabla N(u_1), p_1)_d & \nabla N(u_1)^\top \end{pmatrix} \begin{pmatrix} \delta u \\ \delta p \end{pmatrix}, \\ \delta u(-T) = 0, \quad \delta u(0) = \delta u_n^{(i)}, \end{cases} \quad (57)$$

for each of the $(d-d')$ basis vectors $\delta u_n^{(i)} \in \ker \nabla O(u_1(0)) \subset \mathbb{R}^d$. Here, analogously to (16), we introduced the *adjoint fluctuations*

$$\chi \delta p = \delta \dot{u} + \nabla N(u_1) \delta u, \quad (58)$$

in order to reduce the differential equation of the BVP (57) to first order. Note that the differential equation (57) is equivalent to $H\delta u = 0$ where H is the second variation operator (32) in the continuum limit. Denoting the discrete solution of the BVP (57) for the basis vector $\delta u_n^{(i)}$ as boundary condition by

$$\left(\delta u_1^{(i)}, \dots, \delta u_{n-1}^{(i)}, \delta u_n^{(i)} \right), \quad (59)$$

we can then use the linearity of the corresponding BVPs to expand

$$\begin{aligned}
& \delta^2 S^{(n)} \left(\delta u_0 = 0, \delta u_1, \dots, \delta u_{n-1}, \sum_{i=1}^{d-d'} \beta_i \delta u_n^{(i)} \right) \\
&= \delta^2 S^{(n)} \left(\delta u_0 = 0, \sum_{i=1}^{d-d'} \beta_i \delta u_1^{(i)}, \dots, \sum_{i=1}^{d-d'} \beta_i \delta u_{n-1}^{(i)}, \sum_{i=1}^{d-d'} \beta_i \delta u_n^{(i)} \right) \\
&+ \delta^2 S^{(n)} (\delta u_0 = 0, \delta \tilde{u}_1, \dots, \delta \tilde{u}_{n-1}, \delta u_n = 0),
\end{aligned} \tag{60}$$

for any given boundary condition, which completely separates the inner integral over $\delta \tilde{u}_1, \dots, \delta \tilde{u}_{n-1}$ with Dirichlet 0 boundary conditions as desired. The remaining integral over all boundary conditions (52) is a $d - d'$ dimensional Gaussian integral in β and can easily be evaluated in the continuum limit by noticing that for differentiable curves, the continuum limit of the second variation of the action, written as a quadratic form, is simply

$$\begin{aligned}
\delta^2 S[u, w] &= \frac{1}{2} \int_{-T}^0 dt (\dot{u} + \nabla N(u_1)u, \chi^{-1} [\dot{w} + \nabla N(u_1)w])_d \\
&+ (u, (\nabla \nabla N(u_1), p_1)_d w)_d,
\end{aligned} \tag{61}$$

so from (57), we obtain

$$\begin{aligned}
\delta^2 S [\delta u^{(i)}, \delta u^{(j)}] &= \frac{1}{2} \int_{-T}^0 dt (\delta p^{(j)}, \delta \dot{u}^{(i)} + \nabla N(u_1) \delta u^{(i)})_d \\
&+ (\delta u^{(i)}, (\nabla \nabla N(u_1), p_1)_d \delta u^{(j)})_d \\
&= \frac{1}{2} (\delta u^{(i)}(0), \delta p^{(j)}(0))_d,
\end{aligned} \tag{62}$$

for any two solutions $\delta u^{(i)}, \delta u^{(j)}, 1 \leq i, j \leq d - d'$ of the BVP (57). Here, $\delta p^{(j)}$ of course denotes the adjoint fluctuation (58) for the solution $\delta u^{(j)}$. Therefore, the β -integral in (52) can be evaluated to yield

$$\begin{aligned}
& \int_{\mathbb{R}^{d-d'}} d^{d-d'} \beta \exp \left\{ -\delta^2 S^{(n)} \left(\delta u_0 = 0, \delta u_1, \dots, \delta u_{n-1}, \sum_{i=1}^{d-d'} \beta_i \delta u_n^{(i)} \right) \right\} \\
& \times \exp \left\{ -\frac{1}{2} \sum_{i,j=1}^{d-d'} \beta_i \beta_j (\delta u_n^{(i)}, (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \delta u_n^{(j)})_d \right\} \\
&= \exp \{ \delta^2 S^{(n)}(0, \delta \tilde{u}_1, \dots, \delta \tilde{u}_{n-1}, 0) \} \int_{\mathbb{R}^{d-d'}} d^{d-d'} \beta \\
& \times \exp \left\{ -\frac{1}{2} \sum_{i,j=1}^{d-d'} \beta_i \beta_j (\delta u^{(i)}(0), \delta p^{(j)}(0) + (\nabla \nabla O(u_1(0)), \mathcal{F}_1)_{d'} \delta u^{(j)}(0))_d \right\} \\
&= (2\pi)^{(d-d')/2} (\det B)^{-1/2} \exp \{ -\delta^2 S^{(n)}(0, \delta \tilde{u}_1, \dots, \delta \tilde{u}_{n-1}, 0) \},
\end{aligned} \tag{63}$$

where we abbreviate the $(d - d') \times (d - d')$ -dimensional matrix B with

$$B_{ij} := (\delta u^{(i)}(0), \delta p^{(j)}(0) + (\nabla \nabla O(u_1(0)), \mathcal{F}_1)_{d'} \delta u^{(j)}(0))_{d,ij}. \tag{64}$$

Summing up, at the cost of having to solve $(d - d')$ linear boundary value problems of the form (57) for each of the basis vectors of an arbitrary orthonormal basis of $\ker \nabla O(u_1(t=0)) \subset \mathbb{R}^d$ and consequently evaluating the $(d - d') \times (d - d')$ -dimensional determinant $\det B$, we are left only with Dirichlet 0 boundary conditions $\delta u_0 = 0$ and $\delta u_n = 0$ in the path integral (48). The expression for the PDF becomes

$$\begin{aligned} \rho_O(a) &= (2\pi)^{(d-d')/2} \varepsilon^{-d'/2} [\det B \det (\nabla O(u_{1,n}) \nabla O(u_{1,n})^\top)]^{-1/2} \\ &\times \exp \left\{ \alpha \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \{ -\varepsilon^{-1} S_1(a) \} \\ &\times \lim_{n \rightarrow \infty} (2\pi \Delta t)^{-nd/2} (\det \chi)^{-n/2} \int_{\mathbb{R}^d} \left(\prod_{i=1}^{n-1} d^d(\delta u_i) \right) \\ &\times \exp \{ -\delta^2 S^{(n)}(0, \delta u_1, \dots, \delta u_{n-1}, 0) \}, \end{aligned} \quad (65)$$

where the discrete second variation of the action is given by (49) and evaluated with 0 boundary conditions. Now, we turn to the computation of this remaining integral in the continuum limit. A different approach to avoid having to solve boundary value problems will be discussed afterwards, since, e.g. for the practically relevant case of a large number of spatial dimensions d and a one dimensional observable, it is clearly undesirable to solve $d - 1$ BVPs at each a where the PDF should be evaluated.

3.4. Calculating the fluctuation determinant with Dirichlet 0 boundary conditions

The computation of Gaussian path integrals with Dirichlet boundary conditions such as the one in (65) which we follow here is standard and has been discussed in many textbooks and articles. Historically, it goes back to the works of Cameron and Martin [30] and Montroll [31] and has been popularized in the context of one-dimensional quantum mechanics by Gel'fand and Yaglom [32]. The general d -dimensional case has been treated by Papadopoulos [33] and later multiple times in specific applications, e.g. by Braun and Garg [34] or Daumont *et al* [13]. Here, however, we explicitly keep a general α instead of the mid-point or Stratonovich choice $\alpha = 1/2$ in order to demonstrate the discretization dependence of the result of the limit in the second line of (65), which is only cured by the Jacobian that also depends on the discretization. The discretization dependence of the determinant of finite difference operators in the continuum limit has also been noted, but not analyzed in detail, by Forman [35]. Furthermore, Wissel also derived discretization-dependent Gel'fand-Yaglom formulas for the special case of a one-dimensional Ornstein-Uhlenbeck process [22]. The $\alpha = 0$ case of our intermediate result (94) has also been derived in [36].

The integral in (65) which we want to compute in this section is

$$\begin{aligned} I^{(n),\alpha} &= (2\pi \Delta t)^{-nd/2} (\det \chi)^{-n/2} \\ &\times \int_{\mathbb{R}^d} \left(\prod_{i=1}^{n-1} d^d(\delta u_i) \right) \exp \{ -\delta^2 S^{(n)}(0, \delta u_1, \dots, \delta u_{n-1}, 0) \}, \end{aligned} \quad (66)$$

in the continuum limit $n \rightarrow \infty$. Substituting $\delta u_i = \sqrt{2\Delta t} \delta \tilde{u}_i$ for $i = 1, \dots, n - 1$, this integral can be expressed as

$$I^{(n),\alpha} = (2\pi\Delta t)^{-d/2} (\det \chi)^{-n/2} \pi^{-(n-1)d/2} \times \int_{\mathbb{R}^d} \left(\prod_{i=1}^{n-1} d^d(\delta u_i) \right) \exp \left\{ -(\delta u, H^{(n-1),\alpha} \delta u)_{(n-1)d} \right\}, \quad (67)$$

where the $(n-1)d \times (n-1)d$ block tridiagonal matrix $H^{(n-1),\alpha}$ that can be obtained from (49) is given by

$$\begin{aligned} H_{ii}^{(n-1),\alpha} &= 2\chi^{-1} + \Delta t(2\alpha - 1) [\nabla N_i^\top \chi^{-1} + \chi^{-1} \nabla N_i] \\ &\quad + \Delta t^2 [(\alpha^2 + (1-\alpha)^2) \nabla N_i^\top \chi^{-1} \nabla N_i + (\nabla \nabla N_i, p_i)_d] \\ &=: 2\chi^{-1} + \Delta t R_i + \Delta t^2 S_i, \end{aligned} \quad (68)$$

for $i = 1, \dots, n-1$ on the block diagonal (where $\nabla N_i := \nabla N(u_{1,i})$ and so on) and

$$\begin{aligned} H_{i,i+1}^{(n-1),\alpha} &= -\chi^{-1} + \Delta t [(1-\alpha) \nabla N_i^\top \chi^{-1} - \alpha \chi^{-1} \nabla N_{i+1}] \\ &\quad + \Delta t^2 \alpha (1-\alpha) \nabla N_i^\top \chi^{-1} \nabla N_{i+1} \\ &=: -\chi^{-1} + \Delta t P_i^\top + \Delta t^2 Q_i^\top, \end{aligned} \quad (69)$$

as well as

$$H_{i+1,i}^{(n-1),\alpha} = -\chi^{-1} + \Delta t P_i + \Delta t^2 Q_i, \quad (70)$$

for $i = 1, \dots, n-2$. In principle, the integral (67) could be evaluated numerically by brute force methods, either by simply computing the determinant of the matrix H numerically for large enough n , or by Monte Carlo simulations, as detailed in section 3.1. We will follow both strategies for comparison purposes in our numerical examples in section 4. However, it is immediately clear that a direct numerical calculation of the determinant of $H^{(n-1),\alpha}$ soon becomes prohibitively expensive, in particular for a large number of dimensions d which one encounters when applying the formalism that we developed here to spatially discretized partial differential equations (even though the sparsity and structure of the block tridiagonal matrix $H^{(n-1),\alpha}$ could in principle be exploited here). On the other hand, a Monte Carlo approach is typically slow and provides no analytical insights into the form and contribution of the fluctuations around the instanton. As such, an efficient way to evaluate (67) is needed, and this is conveniently provided by formulas of Gel'fand–Yaglom type.

Here, we follow the notation and derivation strategy of Ossipov [37] in order to derive a Gel'fand–Yaglom like, α -dependent equation for $I^{(n),\alpha}$ in the limit $n \rightarrow \infty$. The basic idea can be explained quickly: we integrate out all δu_i step by step in chronological order. By demanding that the result should be a Gaussian function at each step, we can then obtain recursion relations for the parameters of these Gaussians, which turn into a differential equation in the limit $n \rightarrow \infty$. Hence, define

$$\Phi_1(x) = \exp \left\{ -\left(x, [\chi^{-1} + \Delta t R_1 + (\Delta t)^2 S_1] x \right)_d \right\}, \quad (71)$$

as well as

$$\begin{aligned} \Phi_{k+1}(x) = & \exp \left\{ - \left(x, [\Delta t R_{k+1} + \Delta t^2 S_{k+1}] x \right)_d \right\} \pi^{-d/2} \int_{\mathbb{R}^d} d^d y \\ & \times \exp \left\{ - (x - y, \chi^{-1} [x - y])_d - 2 \left(x, [\Delta t P_k + \Delta t^2 Q_k] y \right)_d \right\} \Phi_k(y), \end{aligned} \quad (72)$$

for $k = 1, \dots, n-1$. Then, we can express $I^{(n),\alpha}$ as

$$I^{(n),\alpha} = (2\pi\Delta t)^{-d/2} (\det \chi)^{-n/2} \Phi_n(0). \quad (73)$$

Now, we insert the general Gaussian ansatz

$$\Phi_k(x) = c_k \exp \left\{ - (x, A_k x)_d - (b_k, x) \right\}, \quad (74)$$

with parameters $c_k > 0$, $A_k \in \mathbb{R}^{d \times d}$ symmetric and positive definite, and $b_k \in \mathbb{R}^d$. Clearly, we have

$$A_1 = \chi^{-1} + \Delta t R_1 + \Delta t^2 S_1, \quad b_1 = 0, \quad c_1 = 1, \quad (75)$$

as initial values for these parameters. Plugging in the ansatz (74) into (72) yields the recursion relations

$$\begin{aligned} A_{k+1} = & \chi^{-1} + \Delta t R_{k+1} + \Delta t^2 S_{k+1} \\ & - (\chi^{-1} - \Delta t P_k - \Delta t^2 Q_k) (\chi^{-1} + A_k)^{-1} (\chi^{-1} - \Delta t P_k^\top - \Delta t^2 Q_k^\top), \end{aligned} \quad (76)$$

(which is also true for $k = 0$ if we define $A_0 = \infty$) as well as

$$b_{k+1} = (\chi^{-1} - \Delta t P_k - \Delta t^2 Q_k) (\chi^{-1} + A_k)^{-1} b_k, \quad (77)$$

and

$$c_{k+1} = c_k [\det (\chi^{-1} + A_k)]^{-1/2} \exp \left\{ \frac{1}{4} (b_k, (\chi^{-1} + A_k)^{-1} b_k)_d \right\}. \quad (78)$$

All of these relation directly follow from applying to (72) the general identity

$$\int_{\mathbb{R}^d} d^d x \exp \left\{ - (x, A x)_d + (b, x)_d \right\} = \left[\det \left(\frac{A}{\pi} \right) \right]^{-1/2} \exp \left\{ \frac{1}{4} (b, A^{-1} b)_d \right\} \quad (79)$$

for a Gaussian integral with source term, which we explicitly state here for later convenience. Since $b_1 = 0$, we immediately obtain $b_k = 0$ for all $k = 1, \dots, n$, such that

$$\begin{aligned} I^{(n),\alpha} = & (2\pi\Delta t)^{-d/2} (\det \chi)^{-n/2} \Phi_n(0) = (2\pi\Delta t)^{-d/2} (\det \chi)^{-n/2} c_n \\ = & (2\pi)^{-d/2} \left[\Delta t^d (\det \chi)^n \prod_{k=1}^{n-1} \det (\chi^{-1} + A_k) \right]^{-1/2}. \end{aligned} \quad (80)$$

Now, we define

$$\chi^{-1} + A_k =: \chi^{-1} Y_{k+1} Y_k^{-1}, \quad k = 1, \dots, n-1. \quad (81)$$

With $A_0 = \infty$, we set $Y_0 = 0 \in \mathbb{R}^{d \times d}$, and we are free to choose Y_1 . Taking

$$Y_1 = \Delta t \chi, \quad (82)$$

the integral $I^{(n),\alpha}$ simply becomes

$$I^{(n),\alpha} = (2\pi)^{-d/2} [\det Y_n]^{-1/2}, \quad (83)$$

with this ansatz. The quantities (Y_k) do in fact possess a well-defined continuum limit, since we absorbed all remaining divergent constants in their definition. It is obvious that the initial values for the continuum limit $Y(t)$ will be

$$Y(-T) = 0, \quad \dot{Y}(-T) = \chi. \quad (84)$$

As for the recursion relation in terms of Y , (76) yields

$$\begin{aligned} A_{k+1} &= \chi^{-1} Y_{k+2} Y_{k+1}^{-1} - \chi^{-1} \\ &= \chi^{-1} + \Delta t R_{k+1} + (\Delta t)^2 S_{k+1} \\ &\quad - (\chi^{-1} - \Delta t P_k - \Delta t^2 Q_k) Y_k Y_{k+1}^{-1} \chi (\chi^{-1} - \Delta t P_k^\top - \Delta t^2 Q_k^\top), \end{aligned} \quad (85)$$

or, sorting by powers of Δt and ignoring terms that will vanish for $\Delta t \rightarrow 0$:

$$\begin{aligned} &\chi^{-1} \frac{Y_{k+2} - 2Y_{k+1} + Y_k}{\Delta t^2} - \frac{1}{\Delta t} [R_{k+1} Y_{k+1} + P_k Y_k + \chi^{-1} Y_k Y_{k+1}^{-1} \chi P_k^\top Y_{k+1}] \\ &- [S_{k+1} Y_{k+1} + Q_k Y_k + \chi^{-1} Y_k Y_{k+1}^{-1} \chi Q_k^\top Y_{k+1} - P_k Y_k Y_{k+1}^{-1} \chi P_k^\top Y_{k+1}] = 0. \end{aligned} \quad (86)$$

The first term clearly converges to $\chi^{-1} \ddot{Y}$ in the continuum limit, but the other two terms require a more careful treatment. The second term in the first line of (86) is given by

$$\begin{aligned} &-\frac{1}{\Delta t} [(2\alpha - 1) (\nabla N_{k+1}^\top \chi^{-1} + \chi^{-1} \nabla N_{k+1}) Y_{k+1} \\ &+ ((1 - \alpha) \chi^{-1} \nabla N_k - \alpha \nabla N_{k+1}^\top \chi^{-1}) Y_k \\ &+ \chi^{-1} Y_k Y_{k+1}^{-1} \chi ((1 - \alpha) \nabla N_k^\top \chi^{-1} - \alpha \chi^{-1} \nabla N_{k+1}) Y_{k+1}]. \end{aligned} \quad (87)$$

Now, we expand

$$Y_{k+1} = Y_k + \Delta t \frac{Y_{k+1} - Y_k}{\Delta t} = Y_k + \Delta t \dot{Y}_k, \quad (88)$$

and use

$$\frac{d}{dt} Y^{-1} = -Y^{-1} \dot{Y} Y^{-1}, \quad (89)$$

such that

$$Y_{k+1}^{-1} = Y_k^{-1} - \Delta t Y_k^{-1} \dot{Y}_k Y_k^{-1}. \quad (90)$$

Inserting these expansions yields the following continuum limit for this term:

$$\begin{aligned} &(1 - \alpha) \chi^{-1} \frac{d}{dt} (\nabla N Y) + (1 - \alpha) \frac{d}{dt} (\nabla N^\top) \chi^{-1} Y - \alpha \nabla N^\top \chi^{-1} \dot{Y} \\ &+ (1 - \alpha) \chi^{-1} \dot{Y} Y^{-1} \chi \nabla N^\top \chi^{-1} Y - \alpha \chi^{-1} \dot{Y} Y^{-1} \nabla N Y. \end{aligned} \quad (91)$$

The remaining terms of (86) are of order 1 in Δt , their limit is

$$\begin{aligned}
& (\alpha^2 - 1) \nabla N^\top \chi^{-1} \nabla N Y - (\nabla \nabla N, p_t)_d Y + (1 - \alpha)^2 \chi^{-1} \nabla N \chi \nabla N^\top \chi^{-1} Y \\
& - \alpha(1 - \alpha) \left[\chi^{-1} \nabla N^2 + (\nabla N^\top)^2 \chi^{-1} \right] Y.
\end{aligned} \tag{92}$$

Summing up, we arrive at the final result

$$\lim_{n \rightarrow \infty} I^{(n), \alpha} = (2\pi)^{d/2} [\det Y(0)]^{-1/2}, \tag{93}$$

for the path integral, where $Y \in \mathbb{R}^{d \times d}$ solves the (in general, for $d > 1$) nonlinear second order matrix differential equation

$$\begin{aligned}
& \chi^{-1} \ddot{Y} + (1 - \alpha) \chi^{-1} \frac{d}{dt} (\nabla N Y) + (1 - \alpha) \frac{d}{dt} (\nabla N^\top) \chi^{-1} Y - \alpha \nabla N^\top \chi^{-1} \dot{Y} \\
& + (1 - \alpha) \chi^{-1} \dot{Y} Y^{-1} \chi \nabla N^\top \chi^{-1} Y - \alpha \chi^{-1} \dot{Y} Y^{-1} \nabla N Y \\
& + (\alpha^2 - 1) \nabla N^\top \chi^{-1} \nabla N Y - (\nabla \nabla N, p_t)_d Y + (1 - \alpha)^2 \chi^{-1} \nabla N \chi \nabla N^\top \chi^{-1} Y \\
& - \alpha(1 - \alpha) \left[\chi^{-1} \nabla N^2 + (\nabla N^\top)^2 \chi^{-1} \right] Y = 0,
\end{aligned} \tag{94}$$

with initial conditions $Y(-T) = 0$, $\dot{Y}(-T) = \chi$. This unwieldy equation does in fact depend on α , and so does the value of $\lim_{n \rightarrow \infty} I^{(n), \alpha}$, but we are free to choose any α from now on in order to bring this equation into a simpler form. Obviously, the choice $\alpha = 1$, which corresponds to a fully implicit discretization of the SDE (33), is advantageous as most terms of (94) will vanish in this case. This leads to

$$\chi^{-1} \ddot{Y} - \nabla N^\top \chi^{-1} \dot{Y} - \chi^{-1} \dot{Y} Y^{-1} \nabla N Y - (\nabla \nabla N, p_t)_d Y = 0, \tag{95}$$

which is still nonlinear, but can be transformed into a symmetric matrix Riccati differential equation for which there exist well-known solution methods (see [38] for an overview). Indeed, setting $Q = Y \dot{Y}^{-1} \chi$, we obtain

$$\dot{Q} = \chi - Q \nabla N^\top - \nabla N Q - Q (\nabla \nabla N, p_t)_d Q, \quad Q(-T) = 0 \in \mathbb{R}^{d \times d}. \tag{96}$$

Depending on the system at hand, it can be numerically or theoretically advantageous to linearize (96) by a Radon transform [39]: defining $Q = \delta U \delta P^{-1}$ with $\delta U, \delta P \in \mathbb{R}^{d \times d}$, we have $\delta U(-T) = 0$ and are free to choose $\delta P(-T) = 1$. Then, by demanding that these matrices satisfy a linear matrix differential equation

$$\frac{d}{dt} \begin{pmatrix} \delta U \\ \delta P \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} \delta U \\ \delta P \end{pmatrix}, \tag{97}$$

and inserting the ansatz into (96), we obtain

$$\frac{d}{dt} \begin{pmatrix} \delta U \\ \delta P \end{pmatrix} = \begin{pmatrix} -\nabla N & \chi \\ (\nabla \nabla N, p_t)_d & \nabla N^\top \end{pmatrix} \begin{pmatrix} \delta U \\ \delta P \end{pmatrix}, \quad \delta U(-T) = 0, \quad \delta P(-T) = 1. \tag{98}$$

Remarkably, by these transformations we obtain a classical, linear Gel'fand–Yaglom formula that is equivalent to $H \delta u = 0$ where H is given by (32), which occurs as a matrix-valued linear first order initial value problem (IVP) in this case and was obtained for the choice of $\alpha = 1$, and not $\alpha = 1/2$. However, we note that linearizing the Riccati equation by this substitution may not be advisable numerically, since the δP equation in (98) is integrated forward in time in this case, but the term $\nabla N^\top \delta P$ on the right-hand side of (98) has a different sign than the drift term

in the original SDE (1). Hence, if the original system is dissipative, the amplitude of δP , and consequently, since it occurs as a forcing term in the respective equation, also the amplitude of δU will grow exponentially in time. The nonlinear Riccati equation (96) does not possess this property, but its nonlinearity is undesirable in the sense that for very large dimensions d , as would be encountered in the spatial discretization of multi-dimensional PDEs, the solution of the linear equation (98) could be *parallelized* trivially over the column vectors of δU and δP .

In order to be able to express our final result for the PDF ρ_O in the second order expansion in terms of the solutions of the BVPs (57) and the Riccati IVP (96), we still have to express

$$\begin{aligned} \lim_{n \rightarrow \infty} I^{(n),1} &= (2\pi)^{-d/2} [\det Y(0)]^{-1/2} \\ &= (2\pi)^{-d/2} [\det Q(0) (\det \chi)^{-1} \det \dot{Y}(0)]^{-1/2} \end{aligned} \quad (99)$$

fully in terms of Q . In order to do this, we calculate

$$\begin{aligned} (\det \chi)^{-1} \det \dot{Y}(0) &= \frac{\det \dot{Y}(0)}{\det \dot{Y}(-T)} = \exp \{ \text{tr} \log \dot{Y}(0) - \text{tr} \log \dot{Y}(-T) \} \\ &= \exp \left\{ \int_{-T}^0 dt \frac{d}{dt} (\text{tr} \log \dot{Y}) \right\} \\ &= \exp \left\{ \int_{-T}^0 dt \text{tr} [\ddot{Y} \dot{Y}^{-1}] \right\} \\ &\stackrel{(94)}{=} \exp \left\{ \int_{-T}^0 dt \text{tr} [\chi (\nabla N^\top \chi^{-1} \dot{Y} + \chi^{-1} \dot{Y} Y^{-1} \nabla N Y \right. \\ &\quad \left. + (\nabla \nabla N, p_t)_d Y) \dot{Y}^{-1}] \right\} \\ &= \exp \left\{ \int_{-T}^0 dt \text{tr} [2 \nabla N + (\nabla \nabla N, p_t)_d Q] \right\}, \end{aligned} \quad (100)$$

where we repeatedly used the cyclicity property of the trace in the last line, as well as in the differentiation in the second line in order to be able to differentiate $\log \dot{Y}$ as if it was a scalar. Putting everything together we obtain the following final expression for the PDF ρ_O of a nonlinear, d' -dimensional observable of the stochastic process described by the d -dimensional SDE (1) in the small noise and continuum limit:

$$\begin{aligned} \rho_O(a) &= (2\pi\varepsilon)^{-d'/2} [\det B \det (\nabla O(u_1(0)) \nabla O(u_1(0))^\top)]^{-1/2} (\det Q(0))^{-1/2} \\ &\quad \times \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt \text{tr} [(\nabla \nabla N(u_1(t)), p_t(t))_d Q(t)] \right\} \\ &\quad \times \exp \{ -\varepsilon^{-1} S_1(a) \}. \end{aligned} \quad (101)$$

The expression which is shown here was derived for $\alpha = 1$ since this choice clearly yields the simplest result based on our previous discussion. To summarize what has been discussed so far, the method which we just introduced consists of three major steps in order to evaluate the complete second order approximation to the PDF ρ_O at each $a \in \mathbb{R}^{d'}$:

- (a) Calculate the instanton trajectory (u_1, p_1) , which is the solution of the minimization problem (18). The observable value a implicitly enters as a boundary condition, leading to

an a -dependent action $S_I(a)$ at the instanton that determines the $\mathcal{O}(e^{\varepsilon^{-1}})$ contribution to the PDF. The instanton then enters as a background field into the differential equations that need to be solved for the prefactor, and thus introduces a -dependence into the prefactor.

- (b) Solve $d - d'$ boundary value problems (57), and evaluate the final time contribution $\det B$ of their solutions.
- (c) Solve a matrix Riccati equation (96) as an initial value problem for Q and evaluate the corresponding integral in (101) along the trajectory as well as the determinant of $Q(t = 0)$.

We want to stress at this point that even though a consistent discretization was crucial in the derivation of (101), all points 1 to 3 from the list given above can numerically be solved using any discretization or integration scheme that one wants to apply. In the next section, we turn to a simpler alternative to (101) that circumvents the possibly large number of boundary value problems in the method outlined so far, and can be derived quickly from our previous discussion.

3.5. Alternative approach without homogenization

While the reduction of the boundary conditions to Dirichlet 0 is desirable from a theoretical point of view in order to be able to connect our result to other studies that evaluate functional determinants for differential operators with such boundary conditions, the necessity to solve a number of boundary value problems which scales linearly with the system dimension d (if a one-dimensional observable, $d' = 1$, is considered) is clearly undesirable from a practical and in particular numerical point of view. Hence, we will derive an alternative, much simpler approach to evaluate the prefactor in this section that does not require the solution of boundary value problems. In fact, the solution of the Riccati equation (96) already contains all necessary information to evaluate the prefactor. In this section, we will directly work with the $\alpha = 1$ discretization which was shown to be the optimal choice in the previous section.

Our starting point is the Gaussian integral (48) for $\alpha = 1$

$$\begin{aligned} \rho_O(a) &= \varepsilon^{-d'/2} \lim_{n \rightarrow \infty} (2\pi\Delta t)^{-nd/2} (\det \chi)^{-n/2} \\ &\times \exp \left\{ \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \{ -\varepsilon^{-1} S_I(a) \} \\ &\times \int_{\mathbb{R}^d} \left(\prod_{j=1}^n d^d(\delta u_j) \right) \delta(\nabla O(u_{1,n}) \delta u_n) \\ &\times \exp \left\{ -\delta^2 S^{(n)}[\delta u] - \frac{1}{2} (\delta u_n, (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \delta u_n)_d \right\}, \end{aligned} \quad (102)$$

with

$$\begin{aligned} \delta^2 S^{(n)}[\delta u] &= \frac{\Delta t}{2} \left(\sum_{i=0}^{n-1} \left[\left(\frac{\delta u_{i+1} - \delta u_i}{\Delta t} + \nabla N(u_{1,i+1}) \delta u_{i+1}, \chi^{-1} [\dots] \right)_d \right. \right. \\ &\quad \left. \left. + (\delta u_i, (\nabla \nabla N(u_{1,i}), p_{1,i})_d \delta u_i)_d \right] \right. \\ &\quad \left. + (\delta u_n, (\nabla \nabla N(u_{1,n}), p_{1,n})_d \delta u_n)_d \right). \end{aligned} \quad (103)$$

Again substituting $\delta u_i = \sqrt{2\Delta t} \delta \tilde{u}_i$, the PDF becomes

$$\begin{aligned}
\rho_O(a) &= \varepsilon^{-d'/2} \exp \left\{ \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \left\{ -\varepsilon^{-1} S_I(a) \right\} \lim_{n \rightarrow \infty} (\det \chi)^{-n/2} \\
&\times \pi^{-nd/2} \int_{\mathbb{R}^d} \left(\prod_{j=1}^n d^d(\delta u_j) \right) \delta(\sqrt{2\Delta t} \nabla O(u_{1,n}) \delta u_n) \\
&\times \exp \left\{ -(\delta u, H^{(n),1} \delta u)_{nd} - \frac{1}{2} (\delta u_n, (\nabla \nabla O(u_{1,n}), \mathcal{F}_I)_{d'} \delta u_n)_d \right\}, \quad (104)
\end{aligned}$$

with the symmetric $nd \times nd$ block tridiagonal matrix $H^{(n),1}$ with diagonal entries

$$\begin{aligned}
H_{ii}^{(n),1} &= 2\chi^{-1} + \Delta t [\nabla N_i^\top \chi^{-1} + \chi^{-1} \nabla N_i] \\
&+ \Delta t^2 [\nabla N_i^\top \chi^{-1} \nabla N_i + (\nabla \nabla N_i, p_i)_d], \quad (105)
\end{aligned}$$

for $i = 1, \dots, n-1$, but

$$\begin{aligned}
H_{nn}^{(n),1} &= \chi^{-1} + \Delta t [\nabla N_n^\top \chi^{-1} + \chi^{-1} \nabla N_n] \\
&+ \Delta t^2 [\nabla N_n^\top \chi^{-1} \nabla N_n + (\nabla \nabla N_n, p_n)_d]. \quad (106)
\end{aligned}$$

The off-diagonal nonzero blocks are

$$H_{i,i+1}^{(n),1} = -\chi^{-1} - \Delta t \chi^{-1} \nabla N_{i+1} = H_{i+1,i}^\top, \quad (107)$$

for $i = 1, \dots, n-1$. Now, the key observation is that the additional δu_n integral that occurs here does not interfere with the way in which we derived the recursion relation for the sequence of Gaussian integral in the previous section. Instead, using the same nomenclature as in section 3.4, the PDF can be written as

$$\begin{aligned}
\rho_O(a) &= \varepsilon^{-d'/2} \exp \left\{ \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \left\{ -\varepsilon^{-1} S_I(a) \right\} \\
&\times \lim_{n \rightarrow \infty} (\det \chi)^{-n/2} \pi^{-d/2} \int_{\mathbb{R}^d} d^d(\delta u_n) \delta(\sqrt{2\Delta t} \nabla O(u_{1,n}) \delta u_n) \\
&\times \exp \left\{ -\Delta t (\delta u_n, (\nabla \nabla O(u_{1,n}), \mathcal{F}_I)_{d'} \delta u_n)_d \right\} \Phi_n(\delta u_n), \quad (108)
\end{aligned}$$

with the function

$$\Phi_n(\delta u_n) = c_n \exp \left\{ -(\delta u_n, A_n \delta u_n) \right\}, \quad (109)$$

resulting from recursive Gaussian integration as discussed previously. Again using (44) for the d' -dimensional δ -function, this can be rewritten as

$$\begin{aligned}
\rho_O(a) &= (2\pi\varepsilon)^{-d'/2} \exp \left\{ \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \left\{ -\varepsilon^{-1} S_I(a) \right\} \\
&\times \lim_{n \rightarrow \infty} (\det \chi)^{-n/2} c_n (2\pi)^{-d'/2} \int_{\mathbb{R}^{d'}} d^{d'} k \pi^{-d/2} \int_{\mathbb{R}^d} d^d(\delta u_n) \\
&\times \exp \left\{ -(\delta u_n, [A_n + \Delta t (\nabla \nabla O(u_{1,n}), \mathcal{F}_I)_{d'}] \delta u_n) \right. \\
&\left. + \sqrt{2\Delta t} i (\nabla O(u_{1,n})^\top k, \delta u_n)_d \right\}. \quad (110)
\end{aligned}$$

The general formula (79) for Gaussian integrals with source term shows that the last δu_n -integral in (110) evaluates to

$$\begin{aligned}
& \pi^{-d/2} \int_{\mathbb{R}^d} d^d(\delta u_n) \exp \left\{ -(\delta u_n, [A_n + \Delta t(\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'}] \delta u_n) \right\} \\
& \times \exp \left\{ \sqrt{2\Delta t} i (\nabla O(u_{1,n})^\top k, \delta u_n)_d \right\} \\
& = [\det (A_n + \Delta t(\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'})]^{-1/2} \\
& \times \exp \left\{ -\frac{1}{2} \left(\nabla O(u_{1,n})^\top k, \left(\frac{A_n}{\Delta t} + (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \right)^{-1} \right. \right. \\
& \left. \left. \times \nabla O(u_{1,n})^\top k \right)_d \right\}, \tag{111}
\end{aligned}$$

so the k -integral in (110) can also easily be evaluated and leads to the final result

$$\begin{aligned}
\rho_O(a) &= (2\pi\varepsilon)^{-d'/2} \exp \left\{ \int_{-T}^0 \text{tr} [\nabla N(u_1(t))] dt \right\} \exp \left\{ -\varepsilon^{-1} S_1(a) \right\} \\
& \times \lim_{n \rightarrow \infty} \left[(\det \chi)^n c_n^{-2} \det (A_n + \Delta t(\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'}) \right. \\
& \left. \times \det \left(\nabla O(u_{1,n}) \left(\frac{A_n}{\Delta t} + (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \right)^{-1} \nabla O(u_{1,n})^\top \right) \right]^{-1/2}. \tag{112}
\end{aligned}$$

By the definitions from section 3.4, we have

$$\begin{aligned}
& (\det \chi)^n c_n^{-2} \det (A_n + \Delta t(\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'}) \\
& = \Delta t^{-d} \det Y_n \det (A_n + \Delta t(\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'}) \\
& = \det Y_n \det \left(\frac{A_n}{\Delta t} + (\nabla \nabla O(u_{1,n}), \mathcal{F}_1)_{d'} \right), \tag{113}
\end{aligned}$$

and the continuum limit of $A_n/\Delta t$ is found from

$$\chi^{-1} + A_n = \chi^{-1} Y_{n+1} Y_n^{-1} = \chi^{-1} (Y_n + \Delta t \dot{Y}_n + \mathcal{O}(\Delta t^2)) Y_n^{-1}, \tag{114}$$

such that

$$\frac{A_n}{\Delta t} \xrightarrow{n \rightarrow \infty} \chi^{-1} \dot{Y}(0) Y(0)^{-1} = Q(0)^{-1}, \tag{115}$$

and, using the same steps as in section 3.4 to express $\dot{Y}(0)$ in terms of Q ,

$$\det Y_n \xrightarrow{n \rightarrow \infty} \det Q(0) \exp \left\{ \int_{-T}^0 dt \text{tr} [2\nabla N + (\nabla \nabla N, p_1)_d Q] \right\}. \tag{116}$$

Plugging these limits into (112) and defining

$$U = 1 + (\nabla \nabla O(u_1(0)), \mathcal{F}_1)_{d'} Q(0), \tag{117}$$

yields the final, and central result of this paper:

$$\rho_O(a) = (2\pi\varepsilon)^{-d'/2} \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt \operatorname{tr} [(\nabla \nabla N(u_I(t)), p_I(t))_d Q(t)] \right\} \\ \times [\det U \det (\nabla O(u_I(0)) Q(0) U^{-1} \nabla O(u_I(0))^\top)]^{-1/2} \exp \{ -\varepsilon^{-1} S_I \}. \quad (118)$$

This equation estimates the complete prefactor for the PDF of a d' -dimensional observable O in the small noise limit in terms of the solution Q of a single matrix Riccati equation

$$\dot{Q} = \chi - Q \nabla N^\top(u_I) - \nabla N(u_I) Q - Q (\nabla \nabla N(u_I), p_I)_d Q, \quad Q(-T) = 0, \quad (119)$$

that can easily be evaluated numerically once the instanton is known, even for large system dimensions d .

Remark 4 It is also possible to derive (118) and (119) based solely on probabilistic methods, without explicit reference to the path integral computations that were utilized above, by adopting the techniques from [29]. Starting from (29), we note that, for suitable functions $f, g : \mathbb{R}^d \rightarrow \mathbb{R}$, the prefactor can be written as

$$Z = \left\langle f(\delta u(0)) \exp \left\{ -\int_{-T}^0 dt g(\delta u(t)) \right\} \right\rangle, \quad (120)$$

where δu is the Gaussian process defined by (30). Expectations of this form can be computed by the Feynman–Kac formula, which, in its forward version, states that

$$Z = \int_{\mathbb{R}^d} d^d v f(v) K(v, 0; 0, -T). \quad (121)$$

Here, the propagator

$$K(v, t; \delta u(-T) = 0, -T) := \left\langle \delta(\delta u(t) - v) \right. \\ \left. \times \exp \left\{ -\int_{-T}^t dt' g(\delta u(t')) \right\} \right\rangle_{\delta u(-T)=0} \quad (122)$$

solves

$$\partial_t K(v, t; 0, -T) = [G_v^\dagger - g(v)] K(v, t; 0, -T), \quad (123)$$

with G_v^\dagger denoting the adjoint of the infinitesimal generator

$$G_v = -(\nabla N(u_I) v, \nabla_v \cdot)_d + \frac{1}{2} \operatorname{tr} [\chi \nabla_v \nabla_v \cdot] \quad (124)$$

of the process δu , and initial condition

$$K(v, -T; 0, -T) = \delta(v). \quad (125)$$

For the SDE (30) and $g(v) = \frac{1}{2} (v, (\nabla \nabla N(u_I), p_I)_d v)_d$, the propagator equation (123) becomes

$$\partial_t K = \operatorname{tr} [\nabla N(u_I)] K + (\nabla N(u_I) v, \nabla_v K)_d + \frac{1}{2} \operatorname{tr} [\chi \nabla_v \nabla_v K] \\ - \frac{1}{2} (v, (\nabla \nabla N(u_I), p_I)_d v)_d K. \quad (126)$$

Inserting the Gaussian ansatz

$$K(v, t; 0, -T) = c \exp \left\{ -\mu(t) - \frac{1}{2} (v, Q^{-1}(t)v)_d \right\} \quad (127)$$

with $\mu : [-T, 0] \rightarrow \mathbb{R}$ and a symmetric matrix $Q : [-T, 0] \rightarrow \mathbb{R}^{d \times d}$ into (126) and sorting by orders of v gives

$$\dot{\mu} = \frac{1}{2} \text{tr} [\chi Q^{-1} - 2 \nabla N(u_1)], \quad (128)$$

$$\dot{Q} = \chi - \nabla N(u_1) Q - Q \nabla N(u_1)^\top - Q (\nabla \nabla N(u_1), p_1)_d Q. \quad (129)$$

We see that this ansatz immediately recovers the differential Riccati equation (119), and the initial condition (125) necessitates $Q(t \rightarrow -T) \rightarrow 0$. Integrating (128) and proceeding as in (100), we find

$$\begin{aligned} \mu(t) - \mu(-T) &= \frac{1}{2} \left(\text{tr} [\log Q(t)] - \text{tr} [\log Q(-T)] \right. \\ &\quad \left. + \int_{-T}^t dt' \text{tr} [(\nabla \nabla N(u_1), p_1)_d Q] \right), \end{aligned} \quad (130)$$

so the propagator (127) becomes

$$\begin{aligned} K(v, t; 0, -T) &= \tilde{c} [\det Q(t)]^{-1/2} \exp \left\{ -\frac{1}{2} \int_{-T}^t dt' \text{tr} [(\nabla \nabla N(u_1), p_1)_d Q] \right. \\ &\quad \left. - \frac{1}{2} (v, Q^{-1}(t)v)_d \right\}, \end{aligned} \quad (131)$$

where all constants were absorbed into \tilde{c} , which, due to the initial condition (125), turns out to be $\tilde{c} = (2\pi)^{-d/2}$. With this expression for K , we obtain from (121):

$$\begin{aligned} Z &= (2\pi)^{-d/2} \varepsilon^{-d'/2} [\det Q(0)]^{-1/2} \\ &\quad \times \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt' \text{tr} [(\nabla \nabla N(u_1), p_1)_d Q] \right\} \int_{\mathbb{R}^d} d^d v \delta(\nabla O(u_1(0))v) \\ &\quad \times \exp \left\{ -\frac{1}{2} (v, [Q^{-1}(0) + (\nabla \nabla O(u_1(0)), \mathcal{F}_1]_{d'}) v)_d \right\}. \end{aligned} \quad (132)$$

The Gaussian integral in the second line can easily be evaluated analogously to the computations in the previous section, and this precisely reproduces (118). We also remark that this prefactor computation method based on the Feynman–Kac equation could immediately be generalized to include higher order fluctuations as discussed for example in [40–42].

4. Examples

In this section we show two examples of low-dimensional SDEs as a proof of concept for the prefactor computation strategy that we developed in the previous section, as well as preliminary results for the application to the stochastic Burgers equation in one spatial dimension. The detailed analysis of the prefactor computation strategy and its results for the Burgers equation and other SPDEs will be the subject of separate, future work.

4.1. One-dimensional gradient system

We start with the example of a one-dimensional SDE

$$\dot{u} + V'(u) = \eta, \quad \langle \eta(t)\eta(t') \rangle = 2\varepsilon\delta(t - t'), \quad (133)$$

where $V : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth potential with a unique, stable and non-degenerate fixed point $\bar{x} \in \mathbb{R}$, such that $V'(\bar{x}) = 0$ and $V''(\bar{x}) > 0$. We consider the SDE (133) on the time interval $[-T, 0]$ with deterministic initial condition $u(-T) = \bar{x}$, such that the process starts at the fixed point of the dynamics. We want to evaluate the PDF ρ_∞ of the stationary distribution of (133) in the small noise limit. This corresponds to the choice $O = \text{id} : \mathbb{R} \rightarrow \mathbb{R}$ in our formalism (with $d = d' = 1$), and the stationary distribution is available via $T \rightarrow \infty$.

From the Fokker–Planck equation

$$\partial_t \rho(x, t) = \partial_x (V'(x)\rho(x, t)) + \varepsilon \partial_{xx} \rho(x, t), \quad (134)$$

for the PDF of the process (133), the stationary distribution is known to be

$$\rho_\infty(x) = \left[\int_{-\infty}^{\infty} dx' \exp \{ -\varepsilon^{-1} V(x') \} \right]^{-1} \exp \{ -\varepsilon^{-1} V(x) \}, \quad (135)$$

which, by applying Laplace's method on the prefactor in the limit $\varepsilon \rightarrow 0$, becomes

$$\rho_\infty(x) = (2\pi\varepsilon)^{-1/2} (V''(\bar{x}))^{1/2} \exp \{ -\varepsilon^{-1} (V(x) - V(\bar{x})) \}. \quad (136)$$

We will reproduce this result, and in particular the prefactor, from our discussion in section 3 now. Note that the linear observable $O = \text{id}$ does not leave any freedom at the right boundary of the time interval, so the BVP determinant $\det B$ from (101) reduces to 1. Similarly, the observable gradient reduces to 1, which means that (101) and (118) are directly seen to coincide and yield

$$\begin{aligned} \rho(x) &= (2\pi\varepsilon)^{-1/2} Q(0)^{-1/2} \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt V'''(u_1(t)) p_1(t) Q(t) \right\} \\ &\quad \times \exp \{ -\varepsilon^{-1} S_1(x) \}, \end{aligned} \quad (137)$$

where Q solves the one-dimensional Riccati equation

$$\dot{Q} = 2 - 2V''(u_1)Q - V'''(u_1)p_1Q^2, \quad Q(-T) = 0. \quad (138)$$

First, we compute the instanton trajectory: for the minimization problem

$$u_1 = \arg \min_{\substack{u(-T)=\bar{x} \\ u(0)=x}} S[u] = \arg \min_{\substack{u(-T)=\bar{x} \\ u(0)=x}} \frac{1}{4} \int_{-T}^0 dt (\dot{u} + V'(u))^2, \quad (139)$$

the instanton equations that we obtain can be written as

$$\begin{cases} \dot{u}_1 + V'(u_1) = 2p_1 \\ \dot{p}_1 - V''(u_1)p_1 = 0 \end{cases} \quad (140)$$

with boundary conditions $u_1(-T) = \bar{x}$, $u_1(0) = x$. Under our assumptions on V and in the limit $T \rightarrow \infty$, these equations are solved by

$$\dot{u}_1 = V'(u_1) = p_1, \quad (141)$$

such that the action at the instanton becomes

$$S_I(x) = \frac{1}{4} \int_{-\infty}^0 dt (\dot{u}_I + V'(u_I))^2 = \int_{-\infty}^0 dt V'(u_I) \dot{u}_I = V(x) - V(\bar{x}), \quad (142)$$

which correctly reproduces the $\mathcal{O}(e^{\varepsilon^{-1}})$ -term in (136). Now, the easiest way to determine the prefactor in this case is to go back to (95) because it is already linear in one dimension. In terms of Y with $Q = 2Y/\dot{Y}$, the PDF can be written as

$$\rho(x) = (2\pi\varepsilon)^{-1/2} Y(0)^{-1/2} \exp \left\{ \int_{-T}^0 dt V''(u_I(t)) \right\} \exp \left\{ -\varepsilon^{-1} S_I(x) \right\}, \quad (143)$$

where Y solves

$$\ddot{Y} - 2(V''(u_I)\dot{Y} + V'''(u_I)p_I Y) = 0, \quad Y(-T) = 0, \quad \dot{Y}(-T) = 2. \quad (144)$$

Using (141), this becomes

$$\ddot{Y} = 2 \frac{d}{dt} (V''(u_I)Y), \quad (145)$$

which can directly be integrated to yield

$$\ddot{Y} = 2 + 2V''(u_I)Y, \quad Y(-T) = 0. \quad (146)$$

Integrating once more, we obtain

$$Y(t) = 2 \exp \left\{ 2 \int_{-T}^t ds V''(u_I(s)) \right\} \int_{-T}^t ds \exp \left\{ -2 \int_{-T}^s d\tau V''(u_I(\tau)) \right\}. \quad (147)$$

The prefactor in (143) can then be evaluated to

$$\begin{aligned} & Y(0)^{-1/2} \exp \left\{ \int_{-T}^0 dt V''(u_I(t)) \right\} \\ &= \left[2 \int_{-T}^0 ds \exp \left\{ -2 \int_{-T}^s d\tau V''(u_I(\tau)) \right\} \right]^{-1/2}. \end{aligned} \quad (148)$$

Since the instanton trajectory stays at the fixed point \bar{x} for an infinite amount of time in the limit $T \rightarrow \infty$, we approximate

$$\int_{-T}^s d\tau V''(u_I(\tau)) \approx V''(\bar{x})(s + T), \quad (149)$$

which, upon insertion in (148), yields

$$\begin{aligned} & Y(0)^{-1/2} \exp \left\{ \int_{-T}^0 dt V''(u_I(t)) \right\} \stackrel{T \rightarrow \infty}{\sim} \\ & \times \left[2 \int_{-T}^0 ds \exp \left\{ -2V''(\bar{x})(s + T) \right\} \right]^{-1/2} \\ &= \left[\frac{1}{V''(\bar{x})} (1 - \exp \{-2V''(\bar{x})T\}) \right]^{-1/2} \xrightarrow{T \rightarrow \infty} (V''(\bar{x}))^{1/2}. \end{aligned} \quad (150)$$

This calculation correctly reproduces the prefactor in (136). Note that in this case, the prefactor is merely a normalization constant that does not depend on x , but we were still able to determine this constant precisely with our method. In contrast, in the numerical examples that we will consider next, the prefactor does depend on the observable value where the PDF is evaluated. First, however, we remark that we can also calculate the prefactor for the one-dimensional gradient example using any $\alpha \in [0, 1]$, with the same result. Indeed, the general, α -dependent Y -equation (94) reduces to

$$\ddot{Y} + 2(1 - 2\alpha)V''(u_1)\dot{Y} - 2\alpha V'''(u_1)V'(u_1)Y - 4\alpha(1 - \alpha)(V''(u_1))^2 Y = 0, \quad (151)$$

with initial conditions $Y(-T) = 0$, $\dot{Y}(-T) = 2$, and the naive approximations $V''(u_1) = V''(\bar{x})$ and $V'(u_1) = 0$ in the ODE give

$$Y(t) = \frac{1}{V''(\bar{x})} \exp\{-2\alpha V''(\bar{x})(t + T)\} (1 - \exp\{-2V''(\bar{x})(t + T)\}), \quad (152)$$

such that the α -dependent terms in the prefactor

$$Y(0)^{-1/2} \exp\left\{\alpha \underbrace{\int_{-T}^0 dt V''(u_1(t))}_{\approx V''(\bar{x})T}\right\} \stackrel{T \rightarrow \infty}{\sim} V''(\bar{x})^{1/2} [1 - \exp\{-2V''(\bar{x})T\}]^{-1/2}, \quad (153)$$

again tend to $V''(\bar{x})^{1/2}$, canceling out any α -dependence.

4.2. Two-dimensional non-gradient system

Here, we consider a two-dimensional, non-gradient SDE with a one-dimensional observable as a second example, which we now treat numerically. Motivated by future applications to stochastic PDEs, we derive our example from the one-dimensional Burgers equation (10), but apart from this motivation, the example has no physical significance and mainly serves as a technical means to demonstrate the method at this point. We transform the non-dimensionalized Burgers equation with periodic boundary conditions on $[0, 2\pi]$ to Fourier space, which gives

$$\frac{d}{dt}\hat{u}_k + \frac{ik}{4\pi} \sum_{l \in \mathbb{Z}} \hat{u}_{k-l}\hat{u}_l + k^2 \hat{u}_k = \hat{\eta}_k, \quad (154)$$

for $k \in \mathbb{Z}$ and $\hat{u}_k \in \mathbb{C}$ the k th Fourier coefficient. Since the velocity field and the forcing are real, their Fourier coefficients fulfill $\hat{u}_{-k} = \hat{u}_k^*$ and $\hat{\eta}_{-k} = \hat{\eta}_k^*$. Now, by arbitrarily setting all Fourier coefficients \hat{u}_k with $|k| \geq 3$ to zero, we obtain the two-dimensional complex SDE

$$\frac{d}{dt} \begin{pmatrix} \hat{u}_1 \\ \hat{u}_2 \end{pmatrix} + \begin{pmatrix} \hat{u}_1 \\ 4\hat{u}_2 \end{pmatrix} + \frac{i}{2\pi} \begin{pmatrix} \hat{u}_1^* \hat{u}_2 \\ \hat{u}_1^2 \end{pmatrix} = \begin{pmatrix} \hat{\eta}_1 \\ \hat{\eta}_2 \end{pmatrix}. \quad (155)$$

Note that this procedure can be interpreted as a Galerkin truncation of the Burgers equation at the $k = 2$ mode. In principle, apart from numerical efficiency considerations, we could put the cutoff at any number of modes.

A further reduction to a two-dimensional real system can be achieved by considering only the antisymmetric parts of these two modes in real space, which corresponds to keeping only the imaginary parts of their Fourier coefficients. Dropping unnecessary constants for convenience, we arrive at the two-dimensional real example

$$\frac{d}{dt} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_1 \\ 4u_2 \end{pmatrix} + \begin{pmatrix} u_1 u_2 \\ -u_1^2 \end{pmatrix} = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}, \quad \langle \eta(t) \eta^\top(t') \rangle = \varepsilon \operatorname{diag}(\chi_1, \chi_2) \delta(t - t'), \quad (156)$$

where u_1 and u_2 are the imaginary parts of the Fourier coefficients \hat{u}_1 and \hat{u}_2 , respectively. This system is non-gradient, dissipative, and possesses only one stable fixed point of the deterministic dynamics at $u_1 = u_2 = 0$. The covariance matrix of the forcing is chosen to be diagonal, as this will be the case for the Fourier transform of a stationary forcing in real space. As a one-dimensional observable, we approximate the gradient

$$\partial_x u(x=0, t=0) = -\frac{1}{\pi} \sum_{k=1}^{\infty} k \cdot \operatorname{Im}(\hat{u}_k(t=0)), \quad (157)$$

from (5) in terms of the two modes, which yields, upon dropping the unnecessary constant,

$$O(u) = -(u_1 + 2u_2), \quad (158)$$

as the linear observable that we will consider in the following.

For our numerical experiments, we took $T = 1$, $\chi_k = k^{-2}$ and $u_0 = 0 \in \mathbb{R}^2$ as the initial value, and considered three different noise strengths $\varepsilon \in \{0.1, 1, 10\}$. For each of the noise strengths, we performed $2 \cdot 10^8$ Monte Carlo simulations of the SDE (156) in order to evaluate the PDF ρ_O at $t = 0$. For these simulations, we used the stochastic Heun scheme, together with an integrating factor for the linear, dissipative terms, with a time step $\Delta t = 5 \cdot 10^{-4}$, corresponding to $n = 2000$ discretization points in time. Figure 1 shows the results of the Monte Carlo runs for the PDF ρ_O , as well as the vector field N for the SDE (156) and the two-dimensional PDF of $u(t=0)$ itself for $\varepsilon = 1$. Furthermore, figure 2 shows the average path of the process conditioned on hitting an observable value of $a = -3.2$ at $t = 0$ for all three ε , compared to the instanton path u_I for that observable value³ [43].

Once the reference PDFs are obtained, in order to apply the methods from section 3, we first need to compute the instanton configurations over a range of relevant observable values a . Note that our instanton approach with pre-factor estimate necessitates only a single computation of the involved terms for all noise strengths ε , as the scaling in ε is given explicitly in the PDF (101) or (118). This is in contrast to Monte Carlo simulations, which have to be performed for every noise strength ε separately.

³ Note that for $\varepsilon = 0.1$ and $\varepsilon = 1$, this observable value is already quite rare, so the ibis method was used to determine the conditional expectation via.

$$\begin{aligned} \langle u(t_0) | O(u(0)) = a \rangle &= \frac{\langle u(t_0) \delta(O(u(0)) - a) \rangle}{\langle \delta(O(u(0)) - a) \rangle} \\ &= u_I(t_0) + \sqrt{\varepsilon} \frac{\left\langle \delta u(t_0) \delta(O(\delta u(0))) \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt (\delta u, (\nabla \nabla N(u_I), p_I)_d \delta u)_d \right\} \right\rangle}{\left\langle \delta(O(\delta u(0))) \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt (\delta u, (\nabla \nabla N(u_I), p_I)_d \delta u)_d \right\} \right\rangle}, \end{aligned}$$

for all $t_0 \in (-T, 0)$, where δu solves the nonlinear SDE (31).

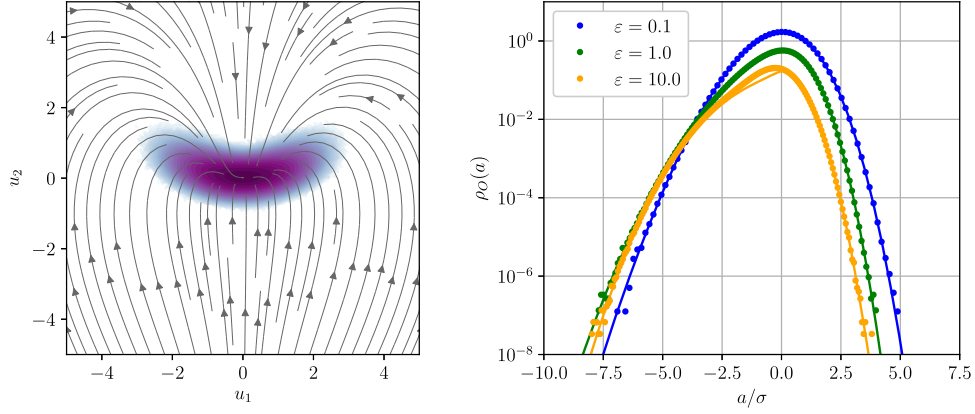


Figure 1. Results of the Monte Carlo simulations of (156) with $2 \cdot 10^8$ samples, and comparison to the instanton estimate including the prefactor Z . The left panel shows the distribution of $u(t=0)$ for $\varepsilon = 1$. The right panel shows the PDFs ρ_O for the observable (158) for different noise strengths ε , scaled by their standard deviation σ . The Monte Carlo results are indicated by the data points, whereas the lines show the result of evaluating (118). We see that for the system at hand, there is an excellent agreement between the Monte Carlo results and the instanton estimate, even at high noise strengths, where slight deviations become visible only at $\varepsilon = 10$. A more precise comparison involving the prefactor itself can be found in figure 4.

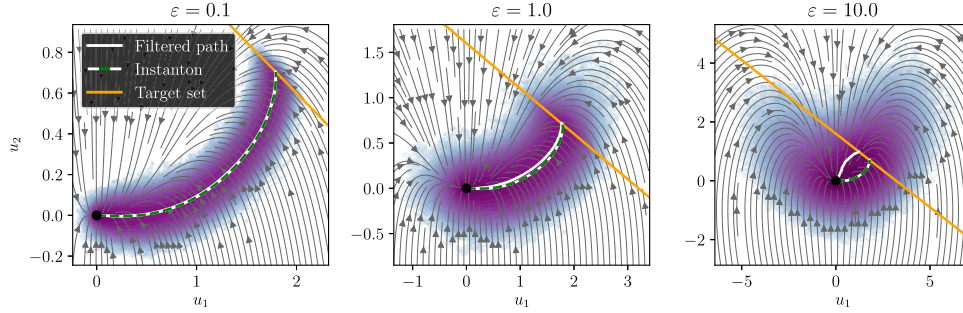


Figure 2. Average paths from Monte Carlo simulations of (156), conditioned on observable values (158) close to $a = -3.2$ (indicated by the orange line) at $t = 0$ for different ε , in comparison to the instanton. The average was taken over 10^4 samples, and the color plot shows the two-dimensional histogram of the data. For a small noise amplitude, the instanton and the filtered path agree well, and we can expect our quadratic approximation to yield good results. At $\varepsilon = 10$, the system is dominated by the noise for this observable value and the instanton path does not provide a good approximation for the filtered path.

For the numerical solution of the instanton optimization problem (18), we incorporated the final time constraint $O(u_f(t=0)) = a$ with a penalty approach and solved the resulting unconstrained optimization problems with the L-BFGS method [44], which is an improvement over the classical Chernykh–Stepanov [45] gradient descent [46]. The same parameters as detailed above were used for the time discretization of the optimization problem, and we checked that variations of the time stepping scheme and time step size do not lead to appreciable differences in the results. After these instanton trajectories, which we computed for 350 equally spaced

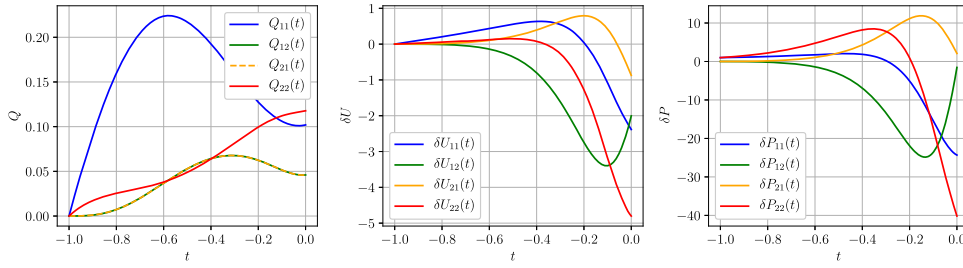


Figure 3. The left panel shows the numerical solution of the Riccati equation (119) for the system (156) and observable (158) at an observable value of $a = -11$. The other two panels show the corresponding solution of the Radon transformed linear equation (98) that corresponds to a classical Gel'fand–Yaglom equation.

values of $a \in [-20, 10]$, have been calculated, we solve the Riccati equation (119) along each of these trajectories in order to evaluate (118). Figure 3 shows a typical solution of the Riccati equation for the system at hand. In order to evaluate the BVP alternative numerically, we have to solve one BVP (57) for each a since the system at hand is two-dimensional with a one-dimensional observable. The observable (158) is linear, so its gradient does not depend on $u_1(0)$, and the boundary value for which we need to solve (57) is given by $\delta u_n^{(1)} = 5^{-1/2}(2, -1)^\top$ for all a . In order to solve (57) numerically, we use a simple shooting method. The PDF that we obtain from (118), including the prefactor, is directly compared to the respective PDFs obtained from direct Monte Carlo simulation of (156) in figure 1. We observe excellent agreement between the instanton estimate and the actual PDFs, and now turn to a more detailed analysis of the numerical results for the prefactor term.

As already mentioned in sections 3.1 and 3.4, there exist further possibilities to individually access the prefactor, the BVP determinant (64) and the functional determinant with Dirichlet 0 boundary conditions $\det H$ from (67) numerically, in order to be able to compare these individual terms to the expressions which we derived. First, the full prefactor Z_ε for $\varepsilon > 0$, defined in (23), is numerically available either by the results of the direct numerical simulations of (1) that we performed, or, in observable ranges that are not sufficiently sampled for a specific ε , by the ibis approach (31). For the quadratic prefactor Z , we can then either simulate (30) for a Monte Carlo approach, solve the BVP (57) and the Riccati equation (119) and evaluate (101), or only solve the Riccati equation and compute Z from (118). The results of these different approaches for the 2-mode system (156) and the ‘velocity gradient’ observable (158) are shown in figure 4. Finally, by simulating (30) with the observable

$$Z^{(0)} = \left\langle \delta(\delta u(0)) \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt (\delta u, (\nabla \nabla N(u_1), p_1)_d \delta u)_d \right\} \right\rangle, \quad (159)$$

we can evaluate the integral (67) with Dirichlet 0 boundary conditions (multiplied by the Jacobian $\exp\{\alpha \int_{-T}^0 dt \operatorname{tr}[\nabla N(u_1)]\}$), in order to compare it to the Gel'fand–Yaglom result (99), as well as a direct numerical computation of the determinant of the $(n-1)d \times (n-1)d$ matrix H as defined by (68) and (69). The quotient of Z and $Z^{(0)}$, as determined from Monte Carlo simulations, should then be given precisely by the BVP determinant $(\det B)^{-1/2}$, which is also shown in figure 4.

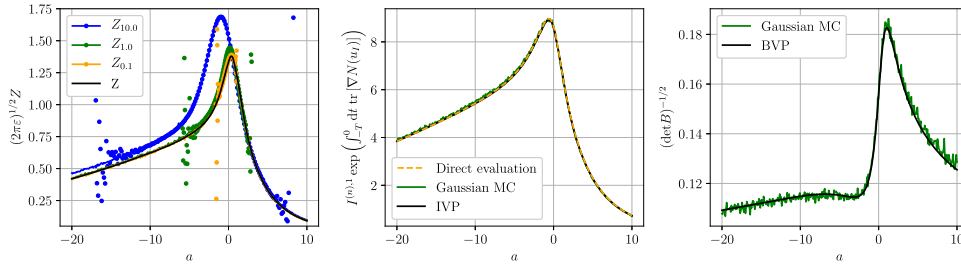


Figure 4. Comparison of Monte Carlo results and our method for the prefactor of the PDF of the linear observable (158) of the two-dimensional SDE (156). The left panel shows the full prefactor Z_ε from (23) as obtained from direct Monte Carlo simulations of (156) at different ε , which is indicated by dots in the figure. The lines of the same color show the results of the ibis method (31) for the same ε 's in order to sample regions that are not accessible by the direct simulations. For the latter, $2 \cdot 10^4$ samples were taken for each observable value. These Monte Carlo results are then compared to the quadratic prefactor Z we obtain from (118). The results of (101) as well as Monte Carlo simulations of (30) for the prefactor Z coincide with this (not shown). The second panel shows the specific contribution of the functional determinant with Dirichlet 0 boundary conditions, together with the Jacobian, to the total prefactor Z , which is either accessible by Monte Carlo simulations of the observable $Z^{(0)}$ from (159), by direct numerical computation of the determinant of the matrix H from (68) and (69), or, of course, by solving the IVP (119). Finally, the last panel to the right shows the contribution of the fluctuations at the right time boundary, which we obtained through the solution of one BVP (57) for each a , and compare to the quotient $Z/Z^{(0)}$ from Monte Carlo simulations.

4.3. Preliminary results for the full Burgers equation

Here, we show preliminary results for the prefactor calculation method from section 3, applied to the full Burgers equation (10) on $[0, 2\pi]$ with periodic boundary conditions at a relatively small spatial resolution $n_x = 64$ (i.e. we have $d = 64$ for this example in the notation of the previous sections). The specific resolution that we used here was chosen arbitrarily; extending the prefactor calculation method to higher spatial resolution poses no conceptual or numerical problems, at least for one-dimensional SPDEs. In this example, we choose the Mexican hat function

$$\chi(x) = -\partial_{xx} \left(\exp \left\{ -\frac{x^2}{2} \right\} \right) = (1 - x^2) \exp \left\{ -\frac{x^2}{2} \right\}, \quad (160)$$

for the large-scale spatial correlation function of the noise, and perform pseudo-spectral Monte Carlo simulations of the Burgers equation (10) at different noise strengths, or, equivalently, at different Reynolds numbers, in order to evaluate the PDF of the gradient of the velocity field (5). The results of these simulations, as well as a comparison to the results of the corresponding instanton and prefactor computations, can be found in figure 5. Note the excellent agreement between the Monte Carlo results and the instanton estimate, both for the full PDF and for the prefactor, even at relatively large ε . As in the previous example, the instanton configurations were computed from a variant of the classical Chernykh–Stepanov algorithm over a range of relevant observable values a , and then, for each a , the Riccati equation (119) was integrated in

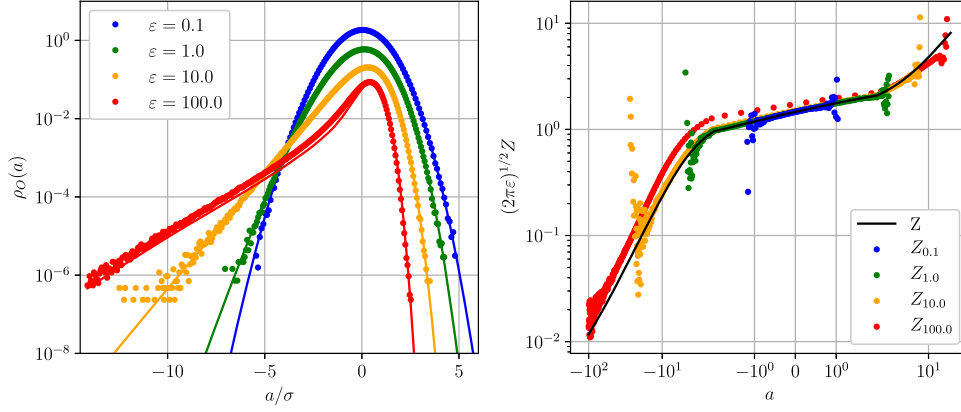


Figure 5. Numerical results for the Burgers equation (10). The left panel shows the PDFs of the gradient observable $O(u) = \partial_x u(x=0, t=0)$ for different noise strengths ε , scaled by their respective standard deviation σ . Using the normalization from [47], the Reynolds number corresponding to these noise strengths is given by $\text{Re} = \varepsilon^{1/3}$. For each ε , we performed $5 \cdot 10^5$ Monte Carlo simulations with a spatial resolution $n_x = 64$ and $n = 1000$ Heun time steps (with integrating factor for the dissipative term) for $T = 1$. The results of these Monte Carlo simulations are indicated by the dots in the left figure, whereas the lines of the same color show the result of evaluating (118). Note that, as in figure 1, deviations of the Monte Carlo results from (118) only become visible at large ε , in this case at $\varepsilon = 100$. The right panel shows the full prefactor Z_ε from (23), as obtained from these Monte Carlo simulations, in comparison to the quadratic prefactor from (118) on a log-log scale.

order to evaluate (118). Due to the fact that we approximate the partial differential equation (10) in this example, the inner products $(\cdot, \cdot)_d$ in (118) and (119) were modified by an additional factor $\Delta x = 2\pi/n_x$ in this case. Concretely, this means that for $Q : [-T, 0] \rightarrow \mathbb{R}^{n_x \times n_x}$, we integrate

$$\dot{Q} = \chi - [\nabla N(u_1)Q + (\nabla N(u_1)Q)^\top] - \Delta x \cdot Q(\nabla \nabla N(u_1), p_1)_d Q, \quad (161)$$

where $\chi \in \mathbb{R}^{n_x \times n_x}$ is a Toeplitz matrix with $\chi_{kl} = \chi((k-l) \cdot \Delta x)$, and $\nabla N(u_1)Q$ as well as $(\nabla \nabla N(u_1), p_1)_d Q$ are evaluated column-wise by means of fast Fourier transforms. The prefactor is then evaluated as

$$Z = (2\pi\varepsilon)^{-1/2} \exp \left\{ -\frac{1}{2} \int_{-T}^0 dt \Delta x \text{tr} [(\nabla \nabla N(u_1(t)), p_1(t))_d Q(t)] \right\} \\ \times [\nabla O(u_1(0))Q(0)\nabla O(u_1(0))^\top]^{-1/2}, \quad (162)$$

where, as $n_x \rightarrow \infty$, the last factor amounts to an evaluation of $\partial_{xy} Q(x=0, y=0, t=0)$ for the linear observable (5).

5. Discussion and outlook

Here, we briefly summarize and discuss the results of this paper and provide an outlook on further related questions. Even though the instanton method is well established in the literature in order to estimate observable PDFs of SDEs in a suitable large deviation limit, general procedures to obtain sharper estimates for these PDFs by including the full prefactor Z at

leading order have not been investigated systematically in this context up until now. For the case of Langevin-type SDEs with additive white-in-time Gaussian noise and unique instanton solutions, we fill this gap with the proposed method. In principle, apart from the unwieldy discretized expressions that we encountered in the derivation of our main result, our approach consists of a straightforward and conceptually simple evaluation of the Gaussian path integral that is obtained by expanding the action to second order around the instanton trajectory. Using a variant of the traditional Gel'fand–Yaglom approach to calculate such path integrals, we were able to reduce the path integral evaluation to the solution of a matrix Riccati differential equation as an initial value problem, which turned out to be possible even for the boundary conditions $\nabla O(u_1(0))\delta u(0) = 0$ on the right boundary of the time interval that we encountered in the specific application of calculating low-dimensional observable PDFs. Numerically, computing the prefactor $Z(a)$ at an observable value $a \in \mathbb{R}^{d'}$ with the proposed method thus amounts to the solution of a single initial value problem of size $d \times d$ in addition to the computation of the instanton itself, which is easily possible for moderately large system dimensions (stemming from the discretization of one-dimensional SPDEs) and in fact much cheaper than the iterative computation of the instanton trajectory. We then proceeded to apply the prefactor calculation method to examples of one-dimensional and two-dimensional SDEs, where the former was treated analytically, whereas, for the latter, we showed detailed numerical results to test the predictions of our prefactor calculation method against Monte Carlo results and direct numerical evaluations of the fluctuation matrix determinant. Afterwards, we showed first results for the important example of the velocity gradient PDF in one-dimensional Burgers turbulence, which already appear quite promising and will be expanded upon in future studies.

In this regard, one of the ultimate questions is what maximum Reynolds numbers can be achieved, and whether this is a possible way to understand intermittency in turbulence. A related question is whether it is possible to recover the high Reynolds number $7/2$ inviscid scaling of the gradient PDF in Burgers turbulence [48, 49] using this approach. Here, on the technical side, it is not clear whether the direct solution of the matrix Riccati equation (119) or the solution of the Radon-transformed linearized system (98) is more advantageous. The linearized system (98) would have the enormous advantage of being ideally suited for parallel calculations, but difficulties may arise due to the appearance of the backward heat equation hidden in the term ∇N^\top . It should be mentioned, however, that the matrix Riccati equation (119) is also amenable to a massive parallel approach [38, 50] or tensor network techniques [51]. The ultimate challenge would be the application of our approach to the full three-dimensional Navier–Stokes equations.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

ORCID iDs

Timo Schorlepp  <https://orcid.org/0000-0002-9143-8854>

Tobias Grafke  <https://orcid.org/0000-0003-0839-676X>

Rainer Grauer  <https://orcid.org/0000-0003-0622-071X>

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